



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:31 AM EDT

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 Full wwPDB X-ray Structure Validation 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

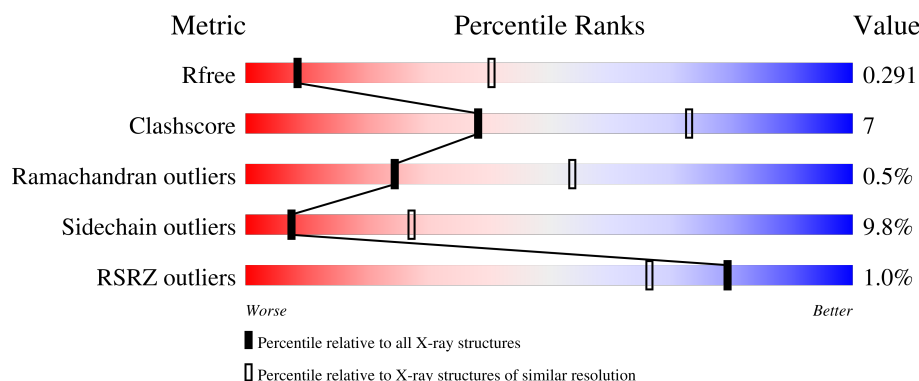
1 Overall quality at a glance

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	40% 47% 13%
1	E	15	40% 47% 13%
2	C	12	8% 83% 8% 8%
2	F	12	92% 8%
3	A	1706	% 77% 14% 6%

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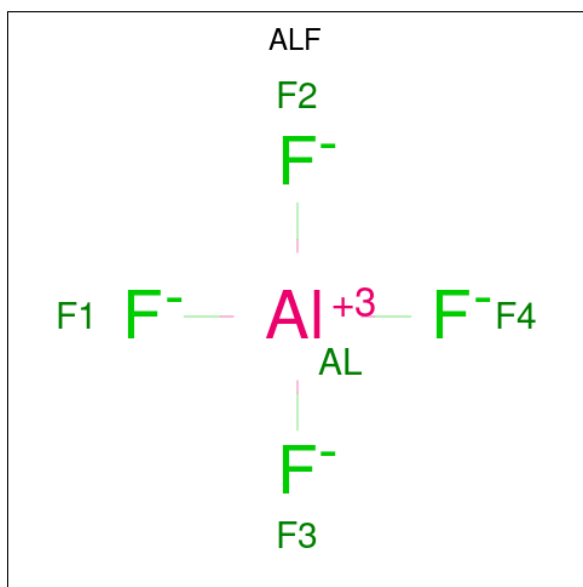
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Chain	Residue	Modelled	Actual	Comment	Reference
D	1992	MET	-	linker	UNP P0A7G6
D	1993	GLY	-	linker	UNP P0A7G6
D	1994	HIS	-	linker	UNP P0A7G6
D	1995	THR	-	linker	UNP P0A7G6
D	1996	THR	-	linker	UNP P0A7G6
D	1997	GLY	-	linker	UNP P0A7G6
D	1998	SER	-	linker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

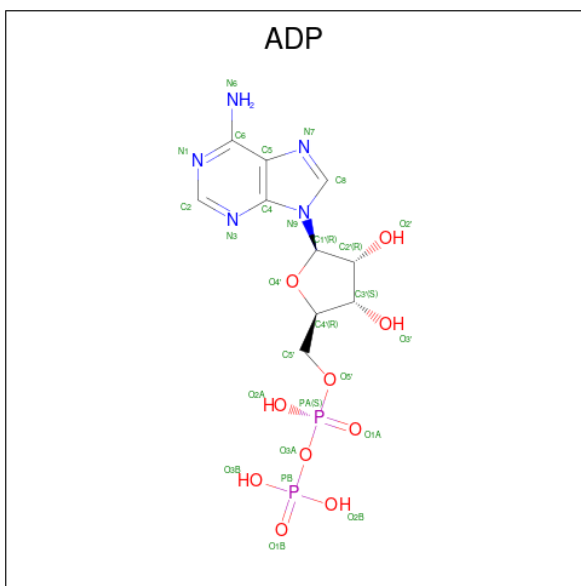
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	Mg	0	0
			5	5		
4	D	5	Total	Mg	0	0
			5	5		

- 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		

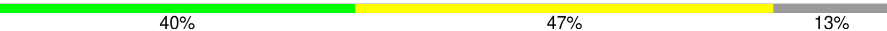
- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

[illegible]

3 Residue-property plots [i](#)

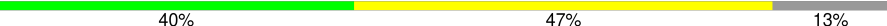
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



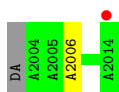
- Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)-3')

Chain E: 



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

Chain C: 



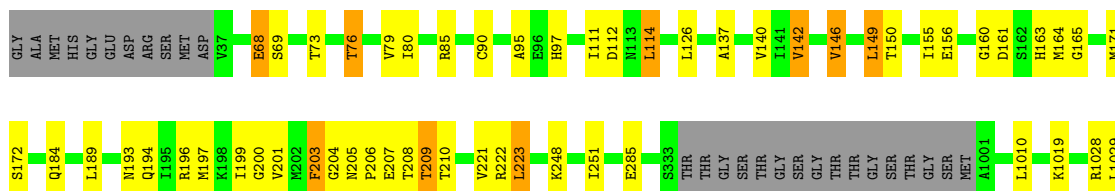
- Molecule 2: DNA (5'-D(*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*A)-3')

Chain F: 



- Molecule 3: Protein recA

Chain A: 



ASN	Q4194	M4035	I3195	M3085	M2197	R2028	R1196	G1030
PRO	I4196	E4068	R3196	M3085	K2198	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	T1208	T1073
	MET	V4079	N3205	T3076	E2207	T2079	T1209	T1076
	PHE	I4080	P3206	T3076	T2208	V2079	T1210	
	GLY	R4085	E3207	V3079	T2209	I2080	K1216	V1079
	N4205	R4085	T3208	I3080	T2210			I1080
		C4090	T3209			R2085		
	T4208	C4090	T3210	M2213			V1221	R1085
	T4209	A4095	N3213	K2216		C2090	R1222	C1090
	T4210	A4095				A2095	L1223	
	G4211	A4096	K3216	V2221		E2096	I1251	A1095
	G4212	H4097		K2222		H2097	P1254	E1096
	N4213	L4114	V3221	L2223		D2100	F1255	H1097
		G4136	R3222	M2236		P2101	K1256	D1100
	K4216	G4136	L3223					P1101
	V4221	V4140	K3248	I2251		I2111	E1285	
	R4222	I4141		P2254		L2114	A1289	T1111
	L4223	V4142	I3251			V2140	N1113	D1112
		V4146	P3254	E2285		I2141	L1114	
	T4251	L4149	Q3261	N2304		V2142	Q1124	
	P4254	E4154	N3269	M2330		V2146	A1125	
	F4270	ILE	E3285	P2331			L1126	
		GLU		N2332		L2149	S1329	
	G4278	GLU		S2333		T2150	N1330	
	V4279	GLU	N3332	THR		E2154	P1331	
		ILE	S3333	THR		I2155	I1141	
	I4284	GLY	THR	GLY			V1140	
	E4285	ASP	THR	SER		G2160	V1142	
		SER	GLY	THR			V1146	
	Y4291	HIS	THR	THR			THR	
	S4292	SER	GLY	GLY			GLY	
	Y4293	HIS	SER	THR			L1149	
	K4294	GLY	THR	GLY			T1150	
		GLY	THR	ALA			GLY	
	G4301	LEU	SER	SER			G1160	
		ALA	MET	GLY			G1165	
	T4306	A4168	SER	SER			GLY	
			GLY	SER			M1171	
	L4309	M4171	GLY	SER			S1172	
	K4310	S4172	ARG	THR			Q1173	
	D4311	Q4173	THR	GLY				
	N4312	R4176	GLY	SER			GLY	
	P4313	K4177	SER	SER			THR	
	E4314	K4177	MET	THR			THR	
	T4315	K4177	SER	SER			GLY	
	A4316	Q4184	A4001	A3001			THR	
			K4019	K3019			THR	
	T4319	L4189	K4019	L3029			THR	
			L4029	D3032			GLY	
	L4328	N4193					THR	
	SER						THR	

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, ADP, MG

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.

All (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
3:A:76:THR:HG21	3:A:142:VAL:HG21	1.50	0.92
3:D:3076:THR:HG21	3:D:3142:VAL:HG21	1.51	0.92
3:D:1076:THR:HG21	3:D:1142:VAL:HG21	1.52	0.92
3:A:1076:THR:HG21	3:A:1142:VAL:HG21	1.49	0.92
1:E:1013:DT:H71	3:D:3199:ILE:HB	1.52	0.91
3:A:3076:THR:HG21	3:A:3142:VAL:HG21	1.52	0.91
3:D:4076:THR:HG21	3:D:4142:VAL:HG21	1.53	0.91
3:A:1193:ASN:HD22	3:A:1194:GLN:H	1.19	0.90
3:D:3193:ASN:HD22	3:D:3194:GLN:H	1.17	0.90
3:A:3193:ASN:HD22	3:A:3194:GLN:H	1.21	0.89
3:A:2304:ASN:HD21	3:D:2304:ASN:CG	1.82	0.88
3:A:193:ASN:HD22	3:A:194:GLN:H	1.20	0.88
3:A:2193:ASN:HD22	3:A:2194:GLN:H	1.18	0.88
3:D:2193:ASN:HD22	3:D:2194:GLN:H	1.22	0.87
3:D:1193:ASN:HD22	3:D:1194:GLN:H	1.21	0.86
3:D:193:ASN:HD22	3:D:194:GLN:H	1.22	0.86
1:E:1013:DT:C7	3:D:3199:ILE:HB	2.07	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:4193:ASN:HD22	3:A:4194:GLN:H	1.25	0.82
3:A:2304:ASN:CG	3:D:2304:ASN:HD21	1.87	0.82
3:D:4193:ASN:HD22	3:D:4194:GLN:H	1.23	0.82
3:D:1068:GLU:HG2	3:D:2216:LYS:HB3	1.62	0.81
3:A:2068:GLU:HG2	3:A:3216:LYS:HB3	1.61	0.80
3:D:194:GLN:HE21	3:D:196:ARG:HH12	1.29	0.79
3:D:1194:GLN:HE21	3:D:1196:ARG:HH12	1.32	0.78
3:A:2194:GLN:HE21	3:A:2196:ARG:HH12	1.32	0.78
3:D:3194:GLN:HE21	3:D:3196:ARG:HH12	1.30	0.78
3:D:3068:GLU:HG2	3:D:4216:LYS:HB3	1.65	0.78
3:A:68:GLU:HG2	3:A:1216:LYS:HB3	1.65	0.77
3:A:3194:GLN:HE21	3:A:3196:ARG:HH12	1.32	0.77
3:A:194:GLN:HE21	3:A:196:ARG:HH12	1.33	0.77
3:A:1194:GLN:HE21	3:A:1196:ARG:HH12	1.33	0.76
3:A:1193:ASN:HD22	3:A:1194:GLN:N	1.83	0.76
3:D:2068:GLU:HG2	3:D:3216:LYS:HB3	1.67	0.75
3:A:2193:ASN:HD22	3:A:2194:GLN:N	1.83	0.75
3:A:2304:ASN:HD21	3:D:2304:ASN:ND2	1.85	0.75
3:D:4194:GLN:HE21	3:D:4196:ARG:HH12	1.34	0.75
3:A:3068:GLU:HG2	3:A:4216:LYS:HB3	1.69	0.75
3:D:2194:GLN:HE21	3:D:2196:ARG:HH12	1.31	0.74
3:A:4194:GLN:HE21	3:A:4196:ARG:HH12	1.32	0.74
3:D:3193:ASN:HD22	3:D:3194:GLN:N	1.84	0.74
3:D:1193:ASN:HD22	3:D:1194:GLN:N	1.84	0.74
3:A:193:ASN:HD22	3:A:194:GLN:N	1.85	0.73
3:D:2193:ASN:HD22	3:D:2194:GLN:N	1.86	0.73
3:D:3197:MET:HE2	3:D:4213:ASN:HD21	1.54	0.72
3:D:193:ASN:HD22	3:D:194:GLN:N	1.87	0.72
3:D:199:ILE:HG22	3:D:200:GLY:H	1.54	0.71
3:D:4193:ASN:HD22	3:D:4194:GLN:N	1.88	0.71
3:A:2304:ASN:ND2	3:D:2304:ASN:HD21	1.87	0.71
3:A:3206:PRO:HG3	3:D:3202:MET:HB2	1.73	0.70
3:D:137:ALA:HB1	3:D:1010:LEU:HB2	1.74	0.70
3:A:3193:ASN:HD22	3:A:3194:GLN:N	1.87	0.70
3:A:2304:ASN:ND2	3:D:2304:ASN:OD1	2.23	0.69
3:A:4193:ASN:HD22	3:A:4194:GLN:N	1.89	0.69
3:A:2171:MET:HE2	3:A:2171:MET:HA	1.75	0.69
3:D:2160:GLY:H	3:D:3173:GLN:HE22	1.38	0.69
3:D:1160:GLY:H	3:D:2173:GLN:HE22	1.41	0.69
3:A:171:MET:HE2	3:A:171:MET:HA	1.76	0.68
3:D:76:THR:CG2	3:D:142:VAL:HG21	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:203:PHE:CG	3:D:204:GLY:N	2.61	0.68
3:A:3171:MET:HA	3:A:3171:MET:HE2	1.75	0.68
3:D:1171:MET:HA	3:D:1171:MET:HE2	1.75	0.68
3:A:164:MET:HE1	3:A:1169:ARG:HD2	1.76	0.67
3:D:171:MET:HA	3:D:171:MET:HE2	1.76	0.67
3:A:3150:THR:OG1	3:A:4176:ARG:HB3	1.94	0.67
3:D:2254:PRO:HG3	6:D:1502:ADP:O2'	1.94	0.67
3:A:4076:THR:CG2	3:A:4142:VAL:HG21	2.25	0.66
3:D:4171:MET:HA	3:D:4171:MET:HE2	1.76	0.66
3:A:1068:GLU:HG2	3:A:2216:LYS:HB3	1.77	0.66
3:D:3171:MET:HE2	3:D:3171:MET:HA	1.77	0.66
3:A:1076:THR:CG2	3:A:1142:VAL:HG21	2.25	0.66
3:A:1171:MET:HA	3:A:1171:MET:HE2	1.77	0.66
1:E:1013:DT:H4'	3:D:4212:GLY:HA2	1.78	0.66
3:A:2304:ASN:OD1	3:D:2304:ASN:ND2	2.27	0.65
3:D:2171:MET:HE2	3:D:2171:MET:HA	1.77	0.65
3:D:2076:THR:CG2	3:D:2142:VAL:HG21	2.26	0.65
3:A:3197:MET:HE2	3:A:4213:ASN:HD21	1.61	0.65
3:A:4171:MET:HE2	3:A:4171:MET:HA	1.78	0.64
3:A:3206:PRO:HG3	3:D:3202:MET:CB	2.26	0.64
3:A:4263:LEU:HG	3:A:4269:ASN:HB2	1.77	0.64
3:A:1160:GLY:H	3:A:2173:GLN:HE22	1.44	0.64
3:D:3076:THR:CG2	3:D:3142:VAL:HG21	2.27	0.64
3:D:4254:PRO:HG3	6:D:3502:ADP:O2'	1.98	0.64
3:A:201:VAL:CG1	3:A:206:PRO:HA	2.28	0.63
3:A:2076:THR:CG2	3:A:2142:VAL:HG21	2.28	0.63
1:B:1010:DT:OP2	3:A:2196:ARG:HD2	1.99	0.62
3:A:2160:GLY:H	3:A:3173:GLN:HE22	1.45	0.62
3:A:3254:PRO:HG3	6:A:2502:ADP:O2'	1.98	0.62
3:D:4076:THR:CG2	3:D:4142:VAL:HG21	2.28	0.62
3:A:166:LEU:HD13	3:A:169:ARG:HH21	1.64	0.62
3:A:3155:ILE:HA	3:A:4177:LYS:HE3	1.82	0.62
3:A:3076:THR:CG2	3:A:3142:VAL:HG21	2.29	0.61
3:A:166:LEU:HD13	3:A:169:ARG:NH2	2.17	0.60
3:D:1199:ILE:HD11	3:D:2164:MET:HB3	1.84	0.60
3:A:3112:ASP:O	3:A:4028:ARG:HG2	2.01	0.60
3:D:2150:THR:OG1	3:D:3176:ARG:HB3	2.02	0.59
3:D:111:ILE:HG22	3:D:1030:GLY:CA	2.34	0.58
3:D:1076:THR:CG2	3:D:1142:VAL:HG21	2.28	0.58
3:A:76:THR:CG2	3:A:142:VAL:HG21	2.27	0.58
3:D:2330:ASN:OD1	3:D:2330:ASN:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2199:ILE:HD11	3:A:3164:MET:HB3	1.84	0.57
3:D:137:ALA:CB	3:D:1010:LEU:HB2	2.34	0.57
3:A:1199:ILE:HD11	3:A:2164:MET:HB3	1.86	0.57
3:A:3111:ILE:HG23	3:A:4029:LEU:HD13	1.87	0.56
3:D:3254:PRO:HG3	6:D:2502:ADP:O2'	2.05	0.56
3:A:2197:MET:HE2	3:A:3213:ASN:HD21	1.71	0.56
3:A:3039:THR:OG1	3:A:3332:ASN:ND2	2.38	0.56
3:A:199:ILE:HD13	3:A:1164:MET:HE2	1.88	0.55
3:A:1197:MET:HE2	3:A:2213:ASN:HD21	1.72	0.55
3:D:150:THR:OG1	3:D:1176:ARG:HB3	2.07	0.54
3:D:1197:MET:HE2	3:D:2213:ASN:HD21	1.73	0.54
3:D:3194:GLN:NE2	3:D:3196:ARG:HH12	2.03	0.54
3:A:1254:PRO:HG3	6:A:502:ADP:O2'	2.08	0.54
1:B:1013:DT:OP2	3:A:3196:ARG:HD2	2.08	0.54
3:A:4261:GLN:OE1	3:A:4269:ASN:ND2	2.38	0.53
1:E:1010:DT:OP2	3:D:2196:ARG:HD2	2.08	0.53
3:A:1199:ILE:HD11	3:A:2164:MET:HE2	1.90	0.53
1:E:1013:DT:H73	3:D:3199:ILE:HB	1.89	0.53
3:D:1254:PRO:HG3	6:D:502:ADP:O2'	2.07	0.53
3:D:111:ILE:HG22	3:D:1030:GLY:HA2	1.91	0.53
3:D:201:VAL:O	3:D:201:VAL:HG13	2.08	0.53
3:A:3124:GLN:HG3	3:A:4021:PHE:CD1	2.44	0.53
3:D:3114:LEU:HD12	3:D:4029:LEU:HD12	1.91	0.53
3:D:203:PHE:CD2	3:D:204:GLY:N	2.77	0.52
3:A:162:SER:C	3:A:163:HIS:CG	2.87	0.52
3:A:159:ILE:HG13	3:A:1177:LYS:HD3	1.91	0.52
3:A:1071:GLY:HA2	6:A:1502:ADP:H5'1	1.91	0.52
3:A:1194:GLN:NE2	3:A:1196:ARG:HH12	2.06	0.52
5:A:4501:ALF:F3	6:A:4502:ADP:O3B	2.18	0.52
3:D:1193:ASN:OD1	3:D:1209:THR:HG23	2.10	0.52
3:D:1071:GLY:HA2	6:D:1502:ADP:H5'1	1.92	0.52
3:D:160:GLY:H	3:D:1173:GLN:HE22	1.58	0.51
3:D:3150:THR:OG1	3:D:4176:ARG:HB3	2.10	0.51
3:A:2071:GLY:HA2	6:A:2502:ADP:H5'1	1.92	0.51
3:D:194:GLN:HE22	3:D:196:ARG:HH22	1.58	0.51
3:A:194:GLN:HE22	3:A:196:ARG:HH22	1.59	0.51
3:A:3202:MET:HB2	3:D:3206:PRO:HG3	1.93	0.50
3:A:2254:PRO:HG3	6:A:1502:ADP:O2'	2.10	0.50
3:D:1194:GLN:NE2	3:D:1196:ARG:HH12	2.06	0.50
3:A:2199:ILE:HD11	3:A:3164:MET:HE2	1.91	0.50
3:A:3254:PRO:HG3	6:A:2502:ADP:HO2'	1.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:68:GLU:HG2	3:D:1216:LYS:CB	2.32	0.50
3:D:3194:GLN:HE22	3:D:3196:ARG:HH22	1.59	0.50
3:D:3155:ILE:HA	3:D:4177:LYS:HE3	1.94	0.50
3:D:3111:ILE:HG23	3:D:4029:LEU:HD13	1.93	0.50
3:A:1080:ILE:HD11	3:A:1142:VAL:HG11	1.93	0.50
3:D:194:GLN:NE2	3:D:196:ARG:HH12	2.03	0.50
3:D:80:ILE:HD11	3:D:142:VAL:HG11	1.94	0.50
3:D:1194:GLN:HE22	3:D:1196:ARG:HH22	1.58	0.50
3:D:2332:ASN:CG	3:D:2333:SER:H	2.19	0.50
3:D:2199:ILE:HD11	3:D:3164:MET:HB3	1.93	0.49
3:A:201:VAL:HG11	3:A:206:PRO:HA	1.94	0.49
3:A:2304:ASN:ND2	3:D:2304:ASN:ND2	2.48	0.49
3:A:3194:GLN:HE22	3:A:3196:ARG:HH22	1.60	0.49
3:A:80:ILE:HD11	3:A:142:VAL:HG11	1.94	0.49
3:D:163:HIS:O	3:D:165:GLY:N	2.45	0.49
3:D:2194:GLN:NE2	3:D:2196:ARG:HH12	2.06	0.49
3:D:3197:MET:HE2	3:D:4213:ASN:ND2	2.25	0.49
3:A:1194:GLN:HE22	3:A:1196:ARG:HH22	1.58	0.49
3:D:201:VAL:HG11	3:D:206:PRO:HB3	1.94	0.49
3:A:3202:MET:CB	3:D:3206:PRO:HG3	2.43	0.49
3:D:2194:GLN:HE22	3:D:2196:ARG:HH22	1.61	0.49
3:A:4194:GLN:HE22	3:A:4196:ARG:HH22	1.60	0.48
3:A:329:SER:O	3:A:330:ASN:HB2	2.13	0.48
3:D:4194:GLN:HE22	3:D:4196:ARG:HH22	1.62	0.48
1:B:1007:DT:H2''	1:B:1008:DT:O5'	2.14	0.48
3:A:4146:VAL:HA	3:A:4149:LEU:HD22	1.96	0.48
3:A:163:HIS:O	3:A:164:MET:C	2.56	0.48
3:D:193:ASN:OD1	3:D:209:THR:HG23	2.13	0.48
3:D:1160:GLY:H	3:D:2173:GLN:NE2	2.08	0.48
3:A:4095:ALA:O	3:A:4097:HIS:HD2	1.96	0.48
3:A:4194:GLN:NE2	3:A:4196:ARG:HH12	2.07	0.48
1:E:1012:DT:OP1	3:D:4172:SER:HB3	2.14	0.47
3:A:3194:GLN:NE2	3:A:3196:ARG:HH12	2.06	0.47
3:D:112:ASP:O	3:D:1028:ARG:HG2	2.13	0.47
3:D:2080:ILE:HD11	3:D:2142:VAL:HG11	1.96	0.47
3:A:194:GLN:NE2	3:A:196:ARG:HH12	2.07	0.47
3:A:2199:ILE:CD1	3:A:3164:MET:HB3	2.45	0.47
3:D:2197:MET:HE2	3:D:3213:ASN:HD21	1.78	0.47
3:D:146:VAL:HA	3:D:149:LEU:HD22	1.96	0.47
3:D:1090:CYS:HB2	3:D:1114:LEU:HD23	1.96	0.47
3:D:2160:GLY:H	3:D:3173:GLN:NE2	2.10	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3193:ASN:OD1	3:D:3209:THR:HG23	2.14	0.47
3:D:1080:ILE:HD11	3:D:1142:VAL:HG11	1.97	0.47
3:A:90:CYS:HB2	3:A:114:LEU:HD23	1.96	0.47
3:A:3193:ASN:OD1	3:A:3209:THR:HG23	2.15	0.47
3:D:2194:GLN:HE21	3:D:2196:ARG:NH1	2.08	0.47
3:D:3080:ILE:HD11	3:D:3142:VAL:HG11	1.97	0.47
3:A:1090:CYS:HB2	3:A:1114:LEU:HD23	1.97	0.47
3:A:2090:CYS:HB2	3:A:2114:LEU:HD23	1.96	0.47
3:A:1193:ASN:OD1	3:A:1209:THR:HG23	2.14	0.47
3:A:2194:GLN:HE22	3:A:2196:ARG:HH22	1.61	0.47
3:A:111:ILE:HG22	3:A:1030:GLY:CA	2.45	0.46
3:A:2193:ASN:OD1	3:A:2209:THR:HG23	2.15	0.46
3:A:2194:GLN:NE2	3:A:2196:ARG:HH12	2.07	0.46
3:D:3194:GLN:HE21	3:D:3196:ARG:NH1	2.06	0.46
3:D:3116:CYS:SG	3:D:4035:MET:HE3	2.56	0.46
3:D:1146:VAL:HA	3:D:1149:LEU:HD22	1.97	0.46
3:D:1201:VAL:C	3:D:1202:MET:HE3	2.41	0.46
3:D:2090:CYS:HB2	3:D:2114:LEU:HD23	1.98	0.46
3:A:71:GLY:HA2	6:A:502:ADP:H5'1	1.96	0.46
3:A:4193:ASN:OD1	3:A:4209:THR:HG23	2.15	0.46
3:D:1095:ALA:O	3:D:1097:HIS:HD2	1.99	0.46
3:D:4090:CYS:HB2	3:D:4114:LEU:HD23	1.96	0.46
3:A:1146:VAL:HA	3:A:1149:LEU:HD22	1.97	0.46
3:A:4080:ILE:HD11	3:A:4142:VAL:HG11	1.98	0.46
3:D:111:ILE:HG22	3:D:1030:GLY:N	2.31	0.46
3:D:3201:VAL:C	3:D:3202:MET:HE3	2.41	0.46
3:A:205:ASN:ND2	3:A:207:GLU:HB2	2.31	0.46
3:A:1201:VAL:C	3:A:1202:MET:HE3	2.41	0.46
3:D:1150:THR:OG1	3:D:2176:ARG:HB3	2.16	0.46
3:D:3090:CYS:HB2	3:D:3114:LEU:HD23	1.96	0.45
3:D:3160:GLY:H	3:D:4173:GLN:HE22	1.64	0.45
3:D:4095:ALA:O	3:D:4097:HIS:HD2	2.00	0.45
3:A:3154:GLU:HA	3:A:3163:HIS:NE2	2.31	0.45
1:B:1006:DT:C2	3:A:1199:ILE:HG23	2.52	0.45
3:A:3080:ILE:HD11	3:A:3142:VAL:HG11	1.98	0.45
3:A:3201:VAL:C	3:A:3202:MET:HE3	2.41	0.45
3:D:4193:ASN:OD1	3:D:4209:THR:HG23	2.16	0.45
3:A:2201:VAL:C	3:A:2202:MET:HE3	2.41	0.45
1:B:1010:DT:H2''	1:B:1011:DT:O5'	2.17	0.45
3:A:194:GLN:NE2	3:A:196:ARG:HH22	2.15	0.45
3:A:2080:ILE:HD11	3:A:2142:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2201:VAL:C	3:D:2202:MET:HE3	2.42	0.45
3:D:194:GLN:NE2	3:D:196:ARG:HH22	2.15	0.45
3:D:2111:ILE:HG23	3:D:3029:LEU:HD13	1.98	0.45
3:A:1160:GLY:H	3:A:2173:GLN:NE2	2.14	0.45
3:D:90:CYS:HB2	3:D:114:LEU:HD23	1.98	0.45
3:D:199:ILE:HG22	3:D:200:GLY:N	2.26	0.45
3:A:2111:ILE:HG23	3:A:3029:LEU:HD13	1.99	0.44
3:A:126:LEU:HD21	3:A:171:MET:HE1	2.00	0.44
3:D:3146:VAL:HA	3:D:3149:LEU:HD22	1.99	0.44
3:D:4194:GLN:NE2	3:D:4196:ARG:HH12	2.08	0.44
3:A:95:ALA:O	3:A:97:HIS:HD2	2.00	0.44
3:A:3095:ALA:O	3:A:3097:HIS:HD2	1.99	0.44
3:D:4221:VAL:HG12	3:D:4223:LEU:HD13	1.99	0.44
3:A:221:VAL:HG12	3:A:223:LEU:HD13	1.99	0.44
3:D:4080:ILE:HD11	3:D:4142:VAL:HG11	1.99	0.44
3:A:1221:VAL:HG12	3:A:1223:LEU:HD13	1.99	0.44
3:A:1095:ALA:O	3:A:1097:HIS:HD2	2.01	0.44
3:A:2146:VAL:HA	3:A:2149:LEU:HD22	2.00	0.44
3:A:3160:GLY:H	3:A:4173:GLN:HE22	1.66	0.44
3:D:1112:ASP:O	3:D:2028:ARG:HG2	2.16	0.44
3:D:1194:GLN:NE2	3:D:1196:ARG:HH22	2.15	0.44
3:D:2221:VAL:HG12	3:D:2223:LEU:HD13	1.99	0.44
1:E:1013:DT:H5'	3:D:4213:ASN:ND2	2.33	0.44
3:A:146:VAL:HA	3:A:149:LEU:HD22	2.00	0.44
3:D:1221:VAL:HG12	3:D:1223:LEU:HD13	2.00	0.44
3:A:1194:GLN:NE2	3:A:1196:ARG:HH22	2.16	0.44
3:A:155:ILE:HA	3:A:1177:LYS:HE3	2.00	0.43
3:A:2221:VAL:HG12	3:A:2223:LEU:HD13	1.99	0.43
3:D:221:VAL:HG12	3:D:223:LEU:HD13	2.00	0.43
3:A:193:ASN:OD1	3:A:209:THR:HG23	2.17	0.43
3:A:2095:ALA:O	3:A:2097:HIS:HD2	2.01	0.43
3:D:4146:VAL:HA	3:D:4149:LEU:HD22	2.00	0.43
1:E:1007:DT:OP2	3:D:1196:ARG:HD2	2.19	0.43
3:A:3293:TYR:CE2	3:A:3294:LYS:HE2	2.53	0.43
3:D:3071:GLY:HA2	6:D:3502:ADP:H5'1	2.01	0.43
3:D:3332:ASN:CG	3:D:3333:SER:N	2.76	0.43
3:D:3221:VAL:HG12	3:D:3223:LEU:HD13	2.00	0.43
1:E:1007:DT:H2''	1:E:1008:DT:O5'	2.18	0.43
3:A:4090:CYS:HB2	3:A:4114:LEU:HD23	2.00	0.43
3:D:2155:ILE:HA	3:D:3177:LYS:HE3	2.00	0.43
3:D:2193:ASN:OD1	3:D:2209:THR:HG23	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3261:GLN:HB2	3:D:3269:ASN:HB3	2.01	0.43
3:D:1124:GLN:HG3	3:D:2021:PHE:CD1	2.54	0.43
3:A:194:GLN:HE21	3:A:196:ARG:NH1	2.09	0.43
3:A:2150:THR:OG1	3:A:3176:ARG:HB3	2.18	0.43
3:D:1256:LYS:NZ	3:D:1329:SER:HB2	2.33	0.43
3:D:3095:ALA:O	3:D:3097:HIS:HD2	2.01	0.43
3:A:3090:CYS:HB2	3:A:3114:LEU:HD23	1.99	0.43
3:D:1080:ILE:HG23	3:D:1090:CYS:SG	2.59	0.43
3:D:1111:ILE:HG23	3:D:2029:LEU:HD13	2.01	0.43
3:A:1126:LEU:HD21	3:A:1171:MET:HE1	2.01	0.43
3:A:2194:GLN:HE21	3:A:2196:ARG:NH1	2.09	0.43
3:D:95:ALA:O	3:D:97:HIS:HD2	2.02	0.43
3:D:2146:VAL:HA	3:D:2149:LEU:HD22	2.01	0.43
3:A:1150:THR:OG1	3:A:2176:ARG:HB3	2.19	0.42
3:A:2124:GLN:HG3	3:A:3021:PHE:CD1	2.54	0.42
3:D:205:ASN:ND2	3:D:207:GLU:HB2	2.34	0.42
3:A:2293:TYR:CE2	3:A:2294:LYS:HE2	2.55	0.42
3:A:4221:VAL:HG12	3:A:4223:LEU:HD13	2.01	0.42
1:E:1006:DT:C2	3:D:1199:ILE:HG23	2.54	0.42
3:A:3221:VAL:HG12	3:A:3223:LEU:HD13	1.99	0.42
3:A:4194:GLN:NE2	3:A:4196:ARG:HH22	2.17	0.42
3:D:1199:ILE:CD1	3:D:2164:MET:HB3	2.49	0.42
3:D:3126:LEU:HD21	3:D:3171:MET:HE1	2.01	0.42
3:A:112:ASP:O	3:A:1028:ARG:HG2	2.20	0.42
3:D:1330:ASN:HB3	3:D:1331:PRO:HD2	2.00	0.42
1:E:1007:DT:C2	3:D:1199:ILE:HD12	2.55	0.42
3:A:1137:ALA:HB1	3:A:2010:LEU:HB2	2.01	0.42
3:A:3194:GLN:NE2	3:A:3196:ARG:HH22	2.17	0.42
3:D:3222:ARG:HG3	3:D:3248:LYS:HB3	2.02	0.42
3:A:3146:VAL:HA	3:A:3149:LEU:HD22	2.02	0.42
3:D:2194:GLN:NE2	3:D:2196:ARG:HH22	2.17	0.42
1:B:1012:DT:H1'	3:A:4169:ARG:HH11	1.85	0.42
3:A:137:ALA:HB1	3:A:1010:LEU:HB2	2.02	0.42
3:A:1256:LYS:NZ	3:A:1329:SER:OG	2.53	0.42
3:A:2126:LEU:HD21	3:A:2171:MET:HE1	2.01	0.42
3:A:3111:ILE:HG22	3:A:4030:GLY:N	2.35	0.42
3:A:3206:PRO:HG3	3:D:3202:MET:HB3	2.00	0.42
3:D:126:LEU:HD21	3:D:171:MET:HE1	2.01	0.41
3:D:1289:ALA:O	3:D:1301:GLY:N	2.51	0.41
3:D:2095:ALA:O	3:D:2097:HIS:HD2	2.02	0.41
3:D:3251:ILE:HD12	3:D:3251:ILE:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:1213:ASN:OD1	3:A:1216:LYS:HE2	2.20	0.41
3:A:2033:ARG:C	3:A:2035:MET:H	2.28	0.41
3:A:3205:ASN:ND2	3:A:3207:GLU:HB2	2.35	0.41
3:A:1293:TYR:CE2	3:A:1294:LYS:HE2	2.56	0.41
3:A:4205:ASN:ND2	3:A:4207:GLU:HB2	2.35	0.41
3:D:1194:GLN:HE21	3:D:1196:ARG:NH1	2.08	0.41
3:D:2100:ASP:HA	3:D:2101:PRO:HD2	1.93	0.41
3:A:2330:ASN:N	3:A:2331:PRO:HD3	2.35	0.41
3:A:3194:GLN:HE21	3:A:3196:ARG:NH1	2.07	0.41
3:A:293:TYR:CE2	3:A:294:LYS:HE2	2.56	0.41
3:D:1126:LEU:HD21	3:D:1171:MET:HE1	2.01	0.41
3:D:4069:SER:HA	6:D:4502:ADP:O3A	2.20	0.41
3:D:4194:GLN:NE2	3:D:4196:ARG:HH22	2.19	0.41
3:D:194:GLN:HE21	3:D:196:ARG:NH1	2.06	0.41
3:A:4261:GLN:HB2	3:A:4269:ASN:HB3	2.03	0.41
3:D:4194:GLN:HE21	3:D:4196:ARG:NH1	2.11	0.41
3:A:160:GLY:H	3:A:1173:GLN:HE22	1.69	0.41
3:A:1205:ASN:ND2	3:A:1207:GLU:HB2	2.36	0.41
2:C:2006:DA:H2'	3:A:3164:MET:SD	2.61	0.41
3:A:1100:ASP:HA	3:A:1101:PRO:HD2	1.94	0.41
3:A:1155:ILE:HA	3:A:2177:LYS:HE3	2.02	0.41
3:A:1199:ILE:CD1	3:A:2164:MET:HB3	2.51	0.41
3:A:2194:GLN:NE2	3:A:2196:ARG:HH22	2.18	0.41
3:A:3213:ASN:OD1	3:A:3216:LYS:HE2	2.21	0.41
3:A:3222:ARG:HG3	3:A:3248:LYS:HB3	2.02	0.41
3:D:222:ARG:HG3	3:D:248:LYS:HB3	2.03	0.41
3:D:1100:ASP:HA	3:D:1101:PRO:HD2	1.94	0.41
3:D:3032:ASP:CG	3:D:3035:MET:HE2	2.46	0.41
3:D:2205:ASN:ND2	3:D:2207:GLU:HB2	2.36	0.41
1:B:1007:DT:OP2	3:A:1196:ARG:HD2	2.21	0.40
1:E:1010:DT:H2''	1:E:1011:DT:O5'	2.21	0.40
3:A:1222:ARG:HG3	3:A:1248:LYS:HB3	2.03	0.40
3:A:4090:CYS:SG	3:A:4140:VAL:HG13	2.61	0.40
3:A:2032:ASP:CG	3:A:2035:MET:HE2	2.46	0.40
3:D:2154:GLU:HA	3:D:2163:HIS:NE2	2.36	0.40
3:D:3205:ASN:ND2	3:D:3207:GLU:HB2	2.36	0.40
1:E:1010:DT:C2	3:D:2199:ILE:HD12	2.56	0.40
3:A:111:ILE:HG22	3:A:1030:GLY:N	2.36	0.40
3:A:2205:ASN:ND2	3:A:2207:GLU:HB2	2.36	0.40
3:D:1293:TYR:CE2	3:D:1294:LYS:HE2	2.56	0.40
3:A:2198:LYS:HG3	3:A:2201:VAL:HG11	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3198:LYS:HG3	3:D:3201:VAL:HG11	2.03	0.40
3:D:4293:TYR:CE2	3:D:4294:LYS:HE2	2.56	0.40

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

All (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
3	D	3269	ASN
3	A	269	ASN
3	A	2165	GLY
3	A	3165	GLY
3	D	1165	GLY
3	D	2165	GLY

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Mol	Chain	Res	Type
3	D	3165	GLY
3	A	1165	GLY
3	A	163	HIS
3	A	330	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

All (248) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	68	GLU
3	A	69	SER
3	A	73	THR
3	A	76	THR
3	A	79	VAL
3	A	85	ARG
3	A	114	LEU
3	A	140	VAL
3	A	142	VAL
3	A	146	VAL
3	A	149	LEU
3	A	155	ILE
3	A	158	GLU
3	A	159	ILE
3	A	163	HIS
3	A	172	SER
3	A	184	GLN
3	A	189	LEU
3	A	197	MET

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Mol	Chain	Res	Type
3	A	199	ILE
3	A	202	MET
3	A	208	THR
3	A	209	THR
3	A	210	THR
3	A	223	LEU
3	A	251	ILE
3	A	285	GLU
3	A	315	THR
3	A	332	ASN
3	A	1019	LYS
3	A	1029	LEU
3	A	1068	GLU
3	A	1069	SER
3	A	1073	THR
3	A	1076	THR
3	A	1079	VAL
3	A	1085	ARG
3	A	1114	LEU
3	A	1140	VAL
3	A	1142	VAL
3	A	1146	VAL
3	A	1149	LEU
3	A	1172	SER
3	A	1184	GLN
3	A	1189	LEU
3	A	1199	ILE
3	A	1202	MET
3	A	1208	THR
3	A	1209	THR
3	A	1210	THR
3	A	1223	LEU
3	A	1251	ILE
3	A	1285	GLU
3	A	1329	SER
3	A	2019	LYS
3	A	2029	LEU
3	A	2068	GLU
3	A	2069	SER
3	A	2073	THR
3	A	2076	THR
3	A	2079	VAL

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Mol	Chain	Res	Type
3	A	2085	ARG
3	A	2114	LEU
3	A	2140	VAL
3	A	2142	VAL
3	A	2146	VAL
3	A	2149	LEU
3	A	2172	SER
3	A	2184	GLN
3	A	2189	LEU
3	A	2199	ILE
3	A	2202	MET
3	A	2208	THR
3	A	2209	THR
3	A	2210	THR
3	A	2223	LEU
3	A	2251	ILE
3	A	2285	GLU
3	A	2332	ASN
3	A	3019	LYS
3	A	3029	LEU
3	A	3068	GLU
3	A	3069	SER
3	A	3073	THR
3	A	3076	THR
3	A	3079	VAL
3	A	3085	ARG
3	A	3114	LEU
3	A	3140	VAL
3	A	3142	VAL
3	A	3146	VAL
3	A	3149	LEU
3	A	3172	SER
3	A	3184	GLN
3	A	3189	LEU
3	A	3199	ILE
3	A	3202	MET
3	A	3208	THR
3	A	3209	THR
3	A	3210	THR
3	A	3223	LEU
3	A	3251	ILE
3	A	3285	GLU

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Mol	Chain	Res	Type
3	A	3315	THR
3	A	3332	ASN
3	A	4019	LYS
3	A	4028	ARG
3	A	4029	LEU
3	A	4068	GLU
3	A	4069	SER
3	A	4073	THR
3	A	4076	THR
3	A	4079	VAL
3	A	4085	ARG
3	A	4114	LEU
3	A	4140	VAL
3	A	4142	VAL
3	A	4146	VAL
3	A	4149	LEU
3	A	4172	SER
3	A	4184	GLN
3	A	4189	LEU
3	A	4208	THR
3	A	4209	THR
3	A	4210	THR
3	A	4223	LEU
3	A	4251	ILE
3	A	4285	GLU
3	D	68	GLU
3	D	69	SER
3	D	73	THR
3	D	76	THR
3	D	79	VAL
3	D	85	ARG
3	D	114	LEU
3	D	140	VAL
3	D	142	VAL
3	D	146	VAL
3	D	149	LEU
3	D	156	GLU
3	D	161	ASP
3	D	172	SER
3	D	184	GLN
3	D	189	LEU
3	D	197	MET

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Mol	Chain	Res	Type
3	D	203	PHE
3	D	208	THR
3	D	209	THR
3	D	210	THR
3	D	223	LEU
3	D	251	ILE
3	D	285	GLU
3	D	1019	LYS
3	D	1029	LEU
3	D	1068	GLU
3	D	1069	SER
3	D	1073	THR
3	D	1076	THR
3	D	1079	VAL
3	D	1085	ARG
3	D	1114	LEU
3	D	1140	VAL
3	D	1142	VAL
3	D	1146	VAL
3	D	1149	LEU
3	D	1172	SER
3	D	1184	GLN
3	D	1189	LEU
3	D	1199	ILE
3	D	1202	MET
3	D	1208	THR
3	D	1209	THR
3	D	1210	THR
3	D	1223	LEU
3	D	1251	ILE
3	D	1285	GLU
3	D	2019	LYS
3	D	2029	LEU
3	D	2068	GLU
3	D	2069	SER
3	D	2073	THR
3	D	2076	THR
3	D	2079	VAL
3	D	2085	ARG
3	D	2114	LEU
3	D	2140	VAL
3	D	2142	VAL

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Mol	Chain	Res	Type
3	D	2146	VAL
3	D	2149	LEU
3	D	2172	SER
3	D	2184	GLN
3	D	2189	LEU
3	D	2199	ILE
3	D	2202	MET
3	D	2208	THR
3	D	2209	THR
3	D	2210	THR
3	D	2223	LEU
3	D	2251	ILE
3	D	2285	GLU
3	D	2330	ASN
3	D	3019	LYS
3	D	3029	LEU
3	D	3068	GLU
3	D	3069	SER
3	D	3073	THR
3	D	3076	THR
3	D	3079	VAL
3	D	3085	ARG
3	D	3114	LEU
3	D	3140	VAL
3	D	3142	VAL
3	D	3146	VAL
3	D	3149	LEU
3	D	3172	SER
3	D	3184	GLN
3	D	3189	LEU
3	D	3199	ILE
3	D	3202	MET
3	D	3208	THR
3	D	3209	THR
3	D	3210	THR
3	D	3223	LEU
3	D	3251	ILE
3	D	3285	GLU
3	D	4019	LYS
3	D	4029	LEU
3	D	4068	GLU
3	D	4069	SER

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Mol	Chain	Res	Type
3	D	4073	THR
3	D	4076	THR
3	D	4079	VAL
3	D	4085	ARG
3	D	4114	LEU
3	D	4140	VAL
3	D	4142	VAL
3	D	4146	VAL
3	D	4149	LEU
3	D	4172	SER
3	D	4184	GLN
3	D	4189	LEU
3	D	4208	THR
3	D	4209	THR
3	D	4210	THR
3	D	4223	LEU
3	D	4251	ILE
3	D	4285	GLU
3	D	4315	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	97	HIS
3	A	173	GLN
3	A	181	ASN
3	A	193	ASN
3	A	194	GLN
3	A	205	ASN
3	A	300	GLN
3	A	304	ASN
3	A	332	ASN
3	A	1097	HIS
3	A	1173	GLN
3	A	1181	ASN
3	A	1193	ASN
3	A	1194	GLN
3	A	1205	ASN
3	A	1300	GLN
3	A	1304	ASN
3	A	1330	ASN
3	A	2097	HIS

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Mol	Chain	Res	Type
3	A	2173	GLN
3	A	2181	ASN
3	A	2193	ASN
3	A	2194	GLN
3	A	2205	ASN
3	A	2300	GLN
3	A	2304	ASN
3	A	3097	HIS
3	A	3124	GLN
3	A	3173	GLN
3	A	3181	ASN
3	A	3193	ASN
3	A	3194	GLN
3	A	3205	ASN
3	A	3300	GLN
3	A	3304	ASN
3	A	3332	ASN
3	A	4097	HIS
3	A	4173	GLN
3	A	4181	ASN
3	A	4193	ASN
3	A	4194	GLN
3	A	4205	ASN
3	A	4300	GLN
3	A	4304	ASN
3	D	97	HIS
3	D	163	HIS
3	D	173	GLN
3	D	181	ASN
3	D	193	ASN
3	D	194	GLN
3	D	205	ASN
3	D	300	GLN
3	D	304	ASN
3	D	1097	HIS
3	D	1173	GLN
3	D	1181	ASN
3	D	1193	ASN
3	D	1194	GLN
3	D	1205	ASN
3	D	1300	GLN
3	D	1304	ASN

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Mol	Chain	Res	Type
3	D	1330	ASN
3	D	2097	HIS
3	D	2173	GLN
3	D	2181	ASN
3	D	2193	ASN
3	D	2194	GLN
3	D	2205	ASN
3	D	2300	GLN
3	D	2304	ASN
3	D	3097	HIS
3	D	3173	GLN
3	D	3181	ASN
3	D	3193	ASN
3	D	3194	GLN
3	D	3205	ASN
3	D	3300	GLN
3	D	3304	ASN
3	D	4097	HIS
3	D	4173	GLN
3	D	4181	ASN
3	D	4193	ASN
3	D	4194	GLN
3	D	4205	ASN
3	D	4213	ASN
3	D	4300	GLN
3	D	4304	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	5,4	28,29,29	1.49	4 (14%)	43,45,45	2.05	11 (25%)
6	ADP	D	2502	5,4	28,29,29	1.63	5 (17%)	43,45,45	1.74	10 (23%)
6	ADP	A	2502	5,4	28,29,29	1.42	4 (14%)	43,45,45	1.79	8 (18%)
6	ADP	A	3502	5,4	28,29,29	1.51	6 (21%)	43,45,45	1.71	8 (18%)
6	ADP	A	1502	5,4	28,29,29	1.60	5 (17%)	43,45,45	1.78	9 (20%)
5	ALF	A	1501	6	4,4,4	1.35	0	-		
6	ADP	A	4502	5,4	28,29,29	1.46	4 (14%)	43,45,45	1.72	10 (23%)
5	ALF	A	501	6	4,4,4	1.41	0	-		
5	ALF	D	501	6	4,4,4	1.42	0	-		
6	ADP	D	3502	5,4	28,29,29	1.53	4 (14%)	43,45,45	1.74	9 (20%)
5	ALF	D	1501	6	4,4,4	1.29	0	-		
6	ADP	D	1502	5,4	28,29,29	1.62	4 (14%)	43,45,45	1.94	10 (23%)
6	ADP	D	4502	5,4	28,29,29	1.56	6 (21%)	43,45,45	1.67	7 (16%)
5	ALF	A	2501	6	4,4,4	1.37	0	-		
5	ALF	A	3501	6	4,4,4	1.31	0	-		
5	ALF	D	4501	6	4,4,4	1.55	0	-		
5	ALF	D	3501	6	4,4,4	1.31	0	-		
6	ADP	D	502	5,4	28,29,29	1.54	5 (17%)	43,45,45	1.64	11 (25%)
5	ALF	A	4501	6	4,4,4	1.49	0	-		
5	ALF	D	2501	6	4,4,4	1.32	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
6	ADP	A	4502	5,4	-	4/16/32/32	0/3/3/3
6	ADP	A	502	5,4	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	D	2502	5,4	-	4/16/32/32	0/3/3/3
6	ADP	D	3502	5,4	-	2/16/32/32	0/3/3/3
6	ADP	A	2502	5,4	-	1/16/32/32	0/3/3/3
6	ADP	D	1502	5,4	-	2/16/32/32	0/3/3/3
6	ADP	A	3502	5,4	-	4/16/32/32	0/3/3/3
6	ADP	D	4502	5,4	-	5/16/32/32	0/3/3/3
6	ADP	D	502	5,4	-	1/16/32/32	0/3/3/3
6	ADP	A	1502	5,4	-	1/16/32/32	0/3/3/3

All (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
6	D	1502	ADP	C5-C4	5.00	1.48	1.39
6	A	4502	ADP	C5-C4	4.97	1.48	1.39
6	A	3502	ADP	C5-C4	4.63	1.47	1.39
6	A	2502	ADP	C5-C4	4.62	1.47	1.39
6	A	1502	ADP	C5-C4	4.53	1.47	1.39
6	A	1502	ADP	PA-O3A	3.99	1.63	1.59
6	D	1502	ADP	PA-O3A	3.48	1.63	1.59
6	D	2502	ADP	PA-O3A	3.23	1.63	1.59
6	A	1502	ADP	C5-N7	-3.17	1.33	1.39
6	D	1502	ADP	C5-C6	3.17	1.49	1.41
6	A	502	ADP	C5-C6	3.07	1.49	1.41
6	A	3502	ADP	PA-O3A	2.87	1.62	1.59
6	A	502	ADP	C8-N7	2.77	1.37	1.31
6	A	4502	ADP	C5-N7	-2.71	1.34	1.39
6	D	2502	ADP	C5-C6	2.67	1.48	1.41
6	D	502	ADP	C5-C6	2.66	1.48	1.41
6	D	4502	ADP	C5-C6	2.63	1.48	1.41
6	D	4502	ADP	C8-N7	2.61	1.36	1.31
6	A	3502	ADP	C5-N7	-2.61	1.34	1.39
6	A	2502	ADP	C5-C6	2.59	1.48	1.41
6	D	2502	ADP	C8-N7	2.59	1.36	1.31
6	D	1502	ADP	C8-N7	2.53	1.36	1.31
6	D	3502	ADP	C8-N7	2.51	1.36	1.31
6	D	502	ADP	C4-N9	-2.50	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1502	ADP	C4-N9	-2.49	1.32	1.37
6	A	2502	ADP	C5-N7	-2.49	1.34	1.39
6	D	3502	ADP	C5-C6	2.46	1.47	1.41
6	D	502	ADP	C5-N7	-2.45	1.34	1.39
6	A	2502	ADP	C8-N7	2.45	1.36	1.31
6	A	4502	ADP	C8-N7	2.42	1.36	1.31
6	A	3502	ADP	C8-N7	2.42	1.36	1.31
6	D	4502	ADP	PA-O3A	2.41	1.62	1.59
6	D	502	ADP	C8-N7	2.39	1.36	1.31
6	A	3502	ADP	C4-N9	-2.33	1.32	1.37
6	D	4502	ADP	C4-N9	-2.28	1.32	1.37
6	A	3502	ADP	C5-C6	2.27	1.47	1.41
6	D	2502	ADP	C5-N7	-2.25	1.35	1.39
6	D	3502	ADP	C5-N7	-2.21	1.35	1.39
6	A	502	ADP	C4-N3	2.14	1.38	1.34
6	A	1502	ADP	C8-N7	2.13	1.35	1.31
6	D	4502	ADP	C5-N7	-2.09	1.35	1.39
6	A	4502	ADP	C5-C6	2.00	1.46	1.41

All (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
6	D	1502	ADP	N3-C4-N9	5.25	136.09	127.17
6	A	502	ADP	N3-C4-N9	5.20	136.01	127.17
6	D	4502	ADP	C5-C4-N3	-5.20	119.56	126.72
6	D	3502	ADP	C5-C4-N3	-5.01	119.82	126.72
6	A	4502	ADP	C5-C4-N3	-5.01	119.82	126.72
6	D	2502	ADP	C5-C4-N3	-4.96	119.89	126.72
6	A	3502	ADP	N3-C4-N9	4.59	134.97	127.17
6	A	2502	ADP	N3-C4-N9	4.57	134.94	127.17
6	D	502	ADP	C5-C4-N3	-4.54	120.46	126.72
6	A	1502	ADP	N3-C4-N9	4.54	134.88	127.17
6	D	3502	ADP	N3-C4-N9	4.40	134.65	127.17
6	A	502	ADP	N3-C2-N1	-4.39	121.93	128.58
6	D	2502	ADP	N3-C4-N9	4.37	134.60	127.17
6	D	4502	ADP	N3-C4-N9	4.29	134.46	127.17
6	A	502	ADP	C2-N3-C4	4.27	122.26	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	4502	ADP	N3-C4-N9	4.26	134.41	127.17
6	D	1502	ADP	C4-C5-N7	-3.98	106.04	110.58
6	A	2502	ADP	C2-N3-C4	3.85	121.24	111.83
6	A	502	ADP	C4-N9-C8	3.84	109.77	105.74
6	D	1502	ADP	C2-N3-C4	3.78	121.06	111.83
6	D	502	ADP	N3-C4-N9	3.75	133.55	127.17
6	A	3502	ADP	C2-N3-C4	3.57	120.55	111.83
6	A	2502	ADP	N3-C2-N1	-3.56	123.19	128.58
6	A	4502	ADP	N3-C2-N1	-3.50	123.29	128.58
6	A	1502	ADP	N3-C2-N1	-3.44	123.38	128.58
6	A	1502	ADP	C2-N3-C4	3.36	120.03	111.83
6	A	3502	ADP	N3-C2-N1	-3.35	123.51	128.58
6	D	2502	ADP	N3-C2-N1	-3.34	123.53	128.58
6	D	2502	ADP	C2-N3-C4	3.20	119.64	111.83
6	D	3502	ADP	N3-C2-N1	-3.15	123.81	128.58
6	A	4502	ADP	C2-N3-C4	3.15	119.52	111.83
6	D	4502	ADP	C2-N3-C4	3.13	119.48	111.83
6	D	3502	ADP	C2-N3-C4	3.08	119.36	111.83
6	D	1502	ADP	C4-N9-C8	3.07	108.96	105.74
6	D	502	ADP	C2-N3-C4	3.05	119.28	111.83
6	D	502	ADP	O4'-C1'-N9	2.99	113.84	108.09
6	D	502	ADP	N3-C2-N1	-2.97	124.09	128.58
6	A	2502	ADP	C4-C5-N7	-2.90	107.26	110.58
6	D	4502	ADP	C4-C5-N7	-2.84	107.33	110.58
6	D	2502	ADP	C2-N1-C6	2.82	123.36	118.73
6	D	1502	ADP	C5-N7-C8	2.80	107.85	103.45
6	D	4502	ADP	C4-N9-C8	2.76	108.64	105.74
6	D	2502	ADP	C4-C5-N7	-2.76	107.42	110.58
6	D	2502	ADP	C4-N9-C8	2.72	108.59	105.74
6	D	3502	ADP	C2-N1-C6	2.71	123.19	118.73
6	D	4502	ADP	N3-C2-N1	-2.71	124.48	128.58
6	A	4502	ADP	C2-N1-C6	2.70	123.16	118.73
6	A	502	ADP	C4-C5-N7	-2.70	107.50	110.58
6	A	1502	ADP	O3'-C3'-C4'	-2.62	103.57	111.08
6	D	3502	ADP	C4-N9-C8	2.62	108.48	105.74
6	A	4502	ADP	O4'-C1'-N9	2.60	113.09	108.09
6	A	1502	ADP	N6-C6-N1	2.60	124.16	118.38
6	A	1502	ADP	O2B-PB-O3A	-2.57	96.03	104.64
6	A	502	ADP	C6-C5-N7	2.57	137.04	132.09
6	A	4502	ADP	C4-C5-N7	-2.55	107.66	110.58
6	D	1502	ADP	N3-C2-N1	-2.53	124.75	128.58
6	A	502	ADP	N9-C8-N7	-2.52	110.37	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	3502	ADP	C4-C5-N7	-2.49	107.74	110.58
6	A	502	ADP	C5-N7-C8	2.45	107.31	103.45
6	A	4502	ADP	C4-N9-C8	2.37	108.23	105.74
6	D	1502	ADP	O2B-PB-O3A	-2.37	96.68	104.64
6	D	502	ADP	C2'-C1'-N9	-2.37	107.41	113.30
6	A	3502	ADP	O2B-PB-O3A	-2.36	96.71	104.64
6	A	4502	ADP	N6-C6-N1	2.35	123.61	118.38
6	D	502	ADP	C4-C5-N7	-2.34	107.90	110.58
6	D	1502	ADP	C6-C5-N7	2.32	136.57	132.09
6	D	4502	ADP	N6-C6-N1	2.27	123.44	118.38
6	D	502	ADP	O2B-PB-O3A	-2.26	97.05	104.64
6	A	3502	ADP	C4-C5-N7	-2.25	108.01	110.58
6	D	2502	ADP	C5-N7-C8	2.21	106.92	103.45
6	D	502	ADP	C2-N1-C6	2.20	122.35	118.73
6	A	502	ADP	C2'-C1'-N9	-2.20	107.85	113.30
6	A	2502	ADP	C4-N9-C8	2.17	108.02	105.74
6	D	2502	ADP	O2B-PB-O3A	-2.17	97.36	104.64
6	D	3502	ADP	C2'-C1'-N9	-2.16	107.95	113.30
6	D	502	ADP	O2A-PA-O1A	2.15	122.44	112.44
6	A	1502	ADP	C4-N9-C8	2.13	107.97	105.74
6	D	1502	ADP	N9-C8-N7	-2.13	110.92	113.94
6	A	502	ADP	O2A-PA-O1A	2.12	122.32	112.44
6	D	3502	ADP	O2B-PB-O3A	-2.12	97.54	104.64
6	A	1502	ADP	C2-N1-C6	2.11	122.19	118.73
6	D	502	ADP	C4-N9-C8	2.11	107.95	105.74
6	A	3502	ADP	C4-N9-C8	2.09	107.94	105.74
6	A	2502	ADP	C5-N7-C8	2.09	106.73	103.45
6	A	3502	ADP	C2-N1-C6	2.06	122.11	118.73
6	D	2502	ADP	O3'-C3'-C4'	-2.05	105.19	111.08
6	A	4502	ADP	C5-N7-C8	2.03	106.65	103.45
6	A	2502	ADP	O2B-PB-O3A	-2.01	97.89	104.64

There are no chirality outliers.

All (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
6	A	4502	ADP	PA-O3A-PB-O2B

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Mol	Chain	Res	Type	Atoms
6	D	3502	ADP	PA-O3A-PB-O2B
6	A	3502	ADP	PA-O3A-PB-O1B
6	A	4502	ADP	O4'-C4'-C5'-O5'
6	A	502	ADP	PA-O3A-PB-O1B
6	A	4502	ADP	PA-O3A-PB-O1B
6	D	1502	ADP	PA-O3A-PB-O1B
6	D	2502	ADP	PA-O3A-PB-O1B
6	A	502	ADP	PA-O3A-PB-O2B
6	A	502	ADP	PA-O3A-PB-O3B
6	A	3502	ADP	PA-O3A-PB-O2B
6	A	3502	ADP	PA-O3A-PB-O3B
6	A	4502	ADP	PA-O3A-PB-O3B
6	D	1502	ADP	PA-O3A-PB-O2B
6	D	2502	ADP	PA-O3A-PB-O2B
6	D	2502	ADP	PA-O3A-PB-O3B
6	D	3502	ADP	PA-O3A-PB-O3B
6	D	4502	ADP	PA-O3A-PB-O2B
6	D	4502	ADP	PA-O3A-PB-O3B
6	D	2502	ADP	O4'-C4'-C5'-O5'
6	D	4502	ADP	C3'-C4'-C5'-O5'
6	A	3502	ADP	O4'-C4'-C5'-O5'

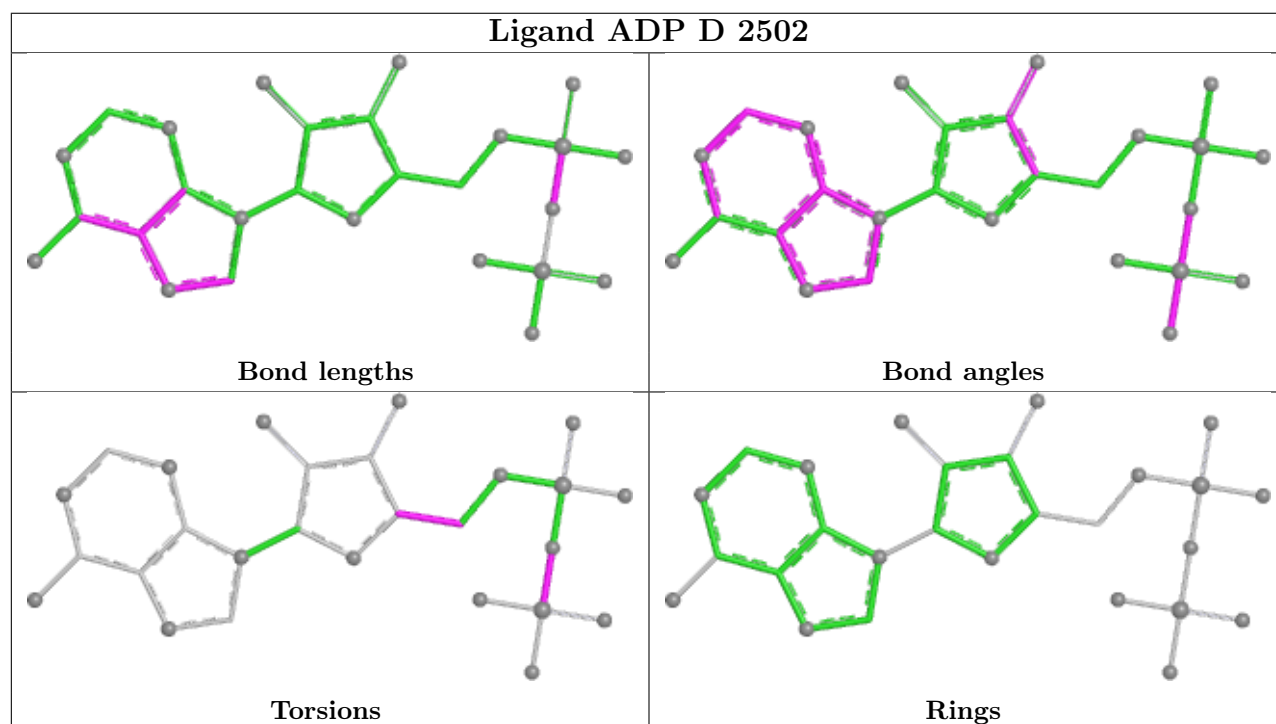
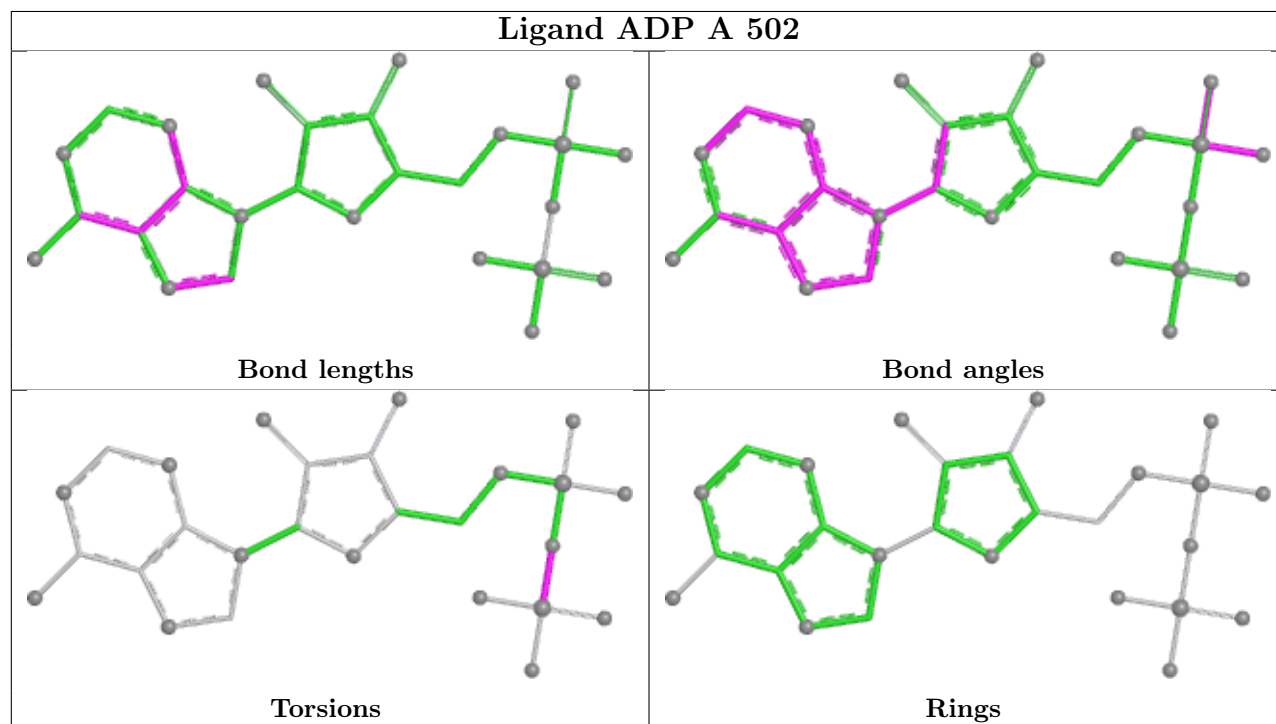
There are no ring outliers.

10 monomers are involved in 15 short contacts:

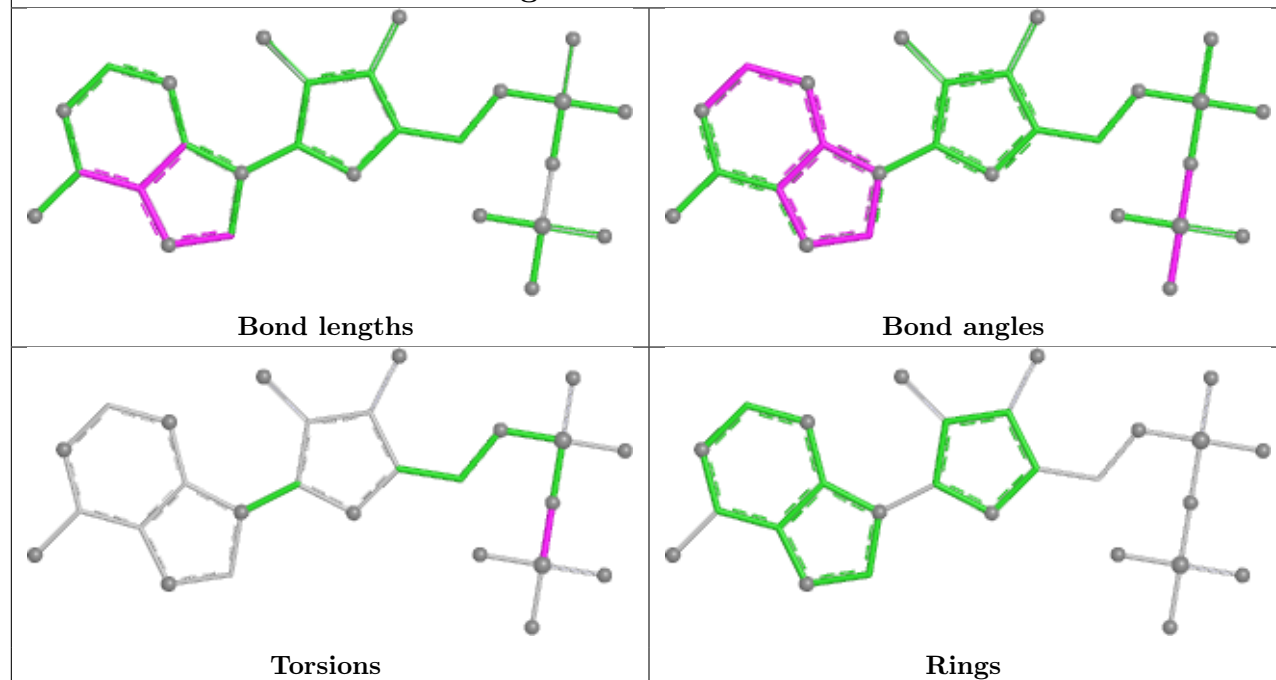
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	502	ADP	2	0
6	D	2502	ADP	1	0
6	A	2502	ADP	3	0
6	A	1502	ADP	2	0
6	A	4502	ADP	1	0
6	D	3502	ADP	2	0
6	D	1502	ADP	2	0
6	D	4502	ADP	1	0
6	D	502	ADP	1	0
5	A	4501	ALF	1	0

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.

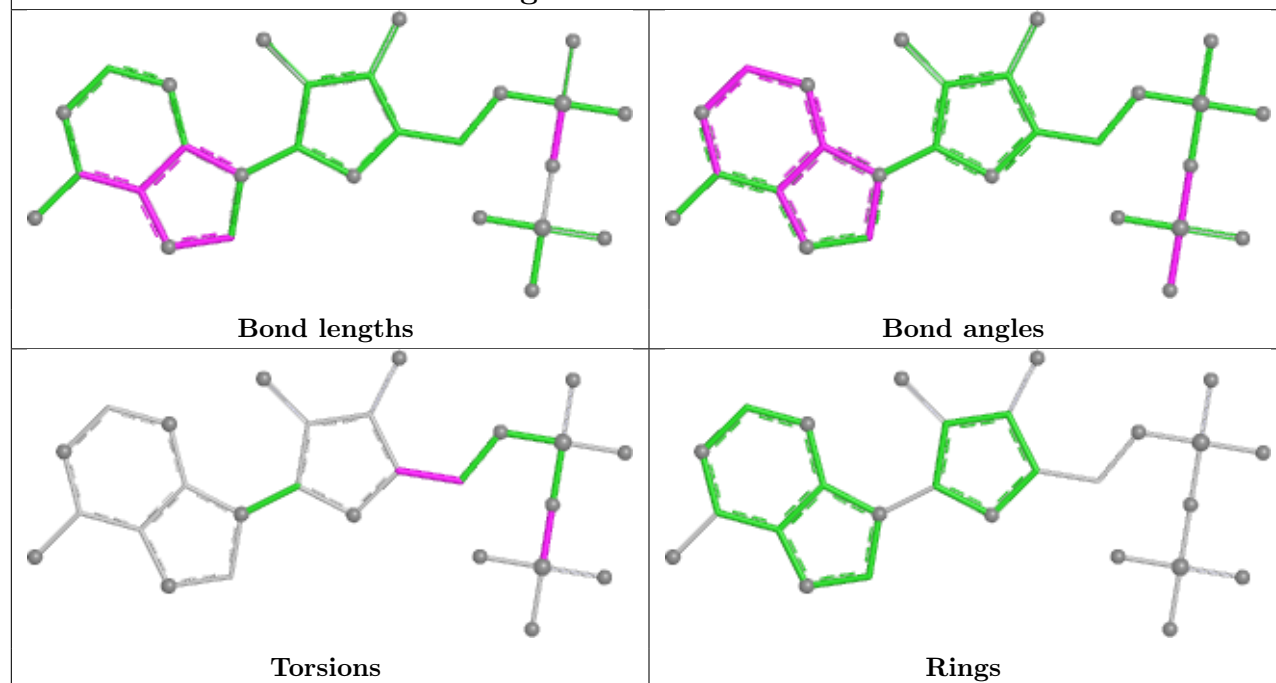
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

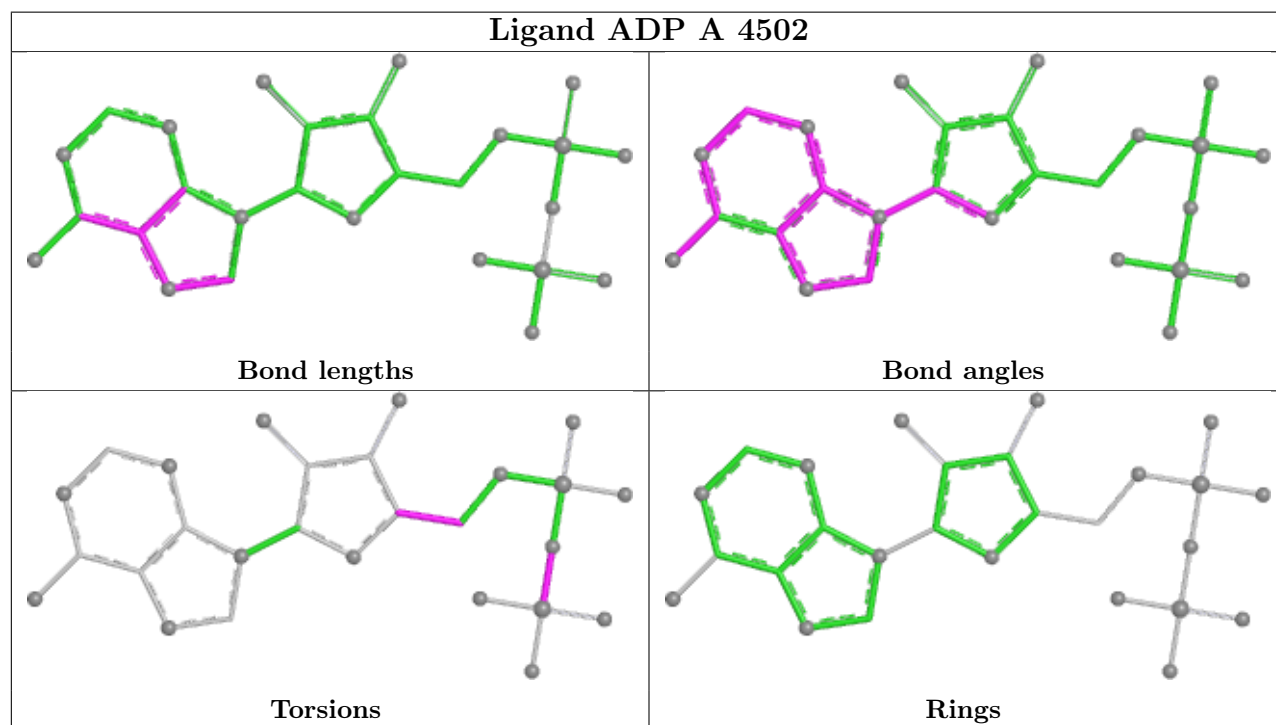
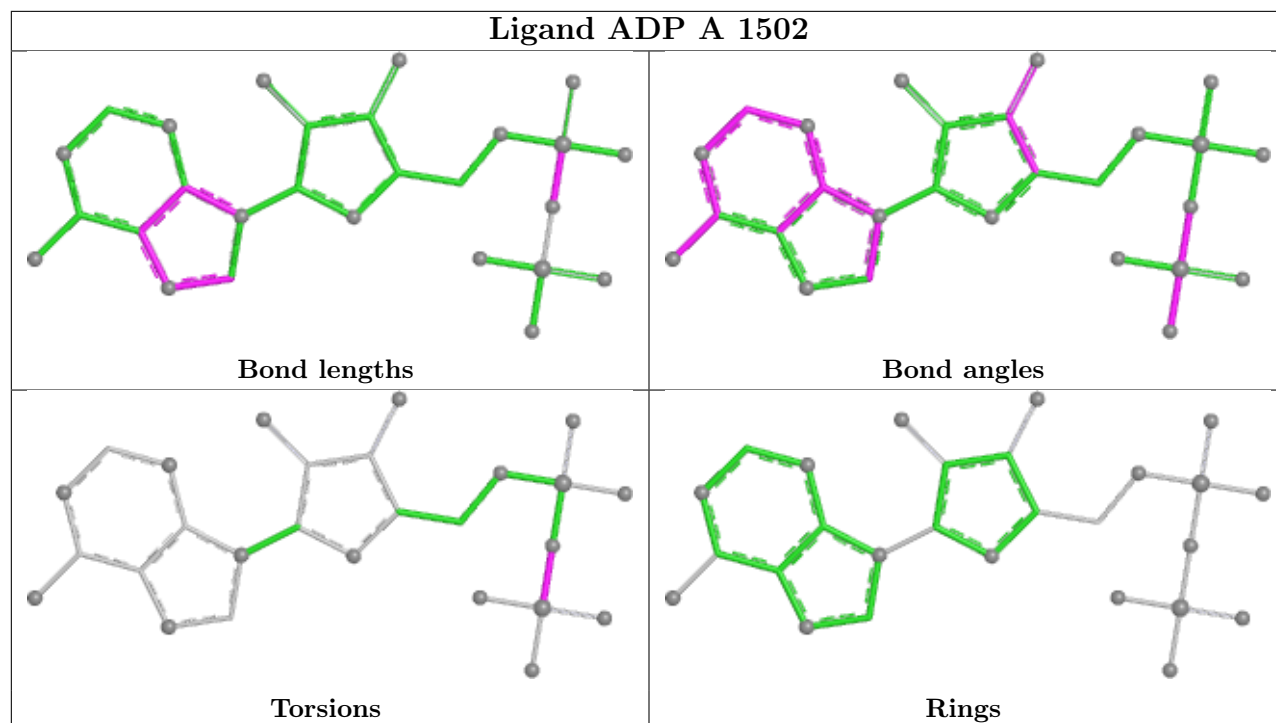


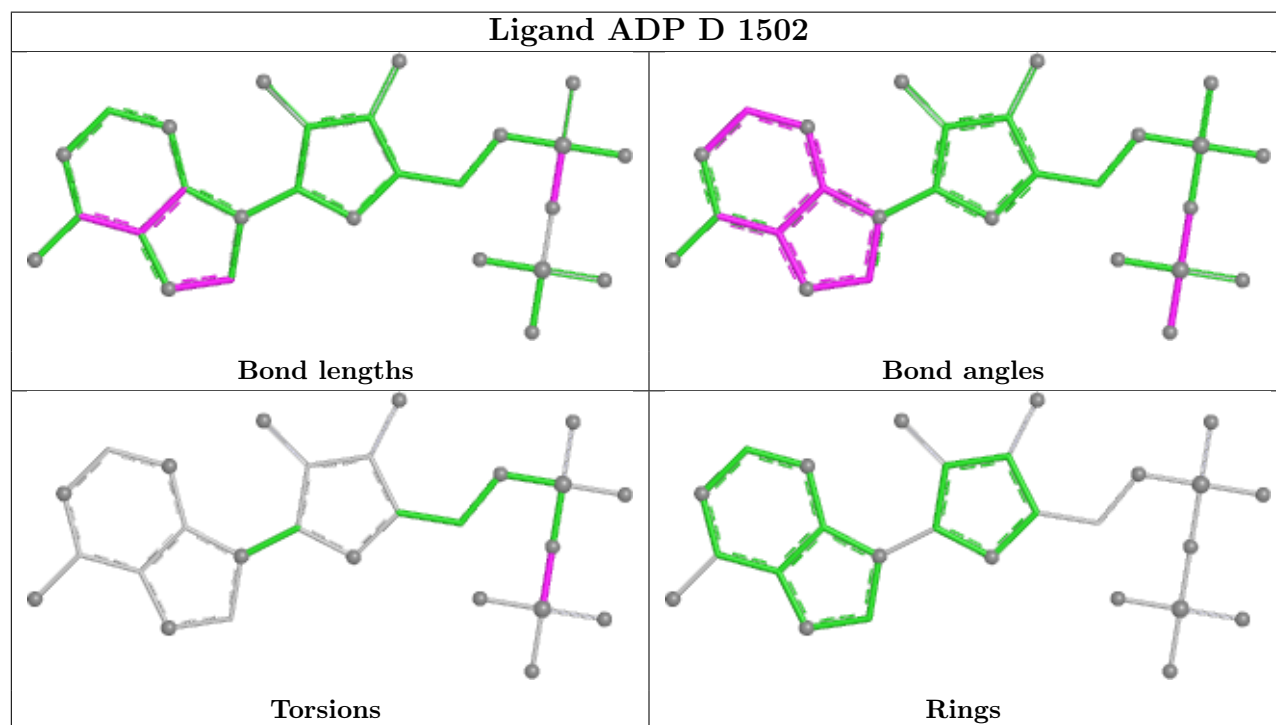
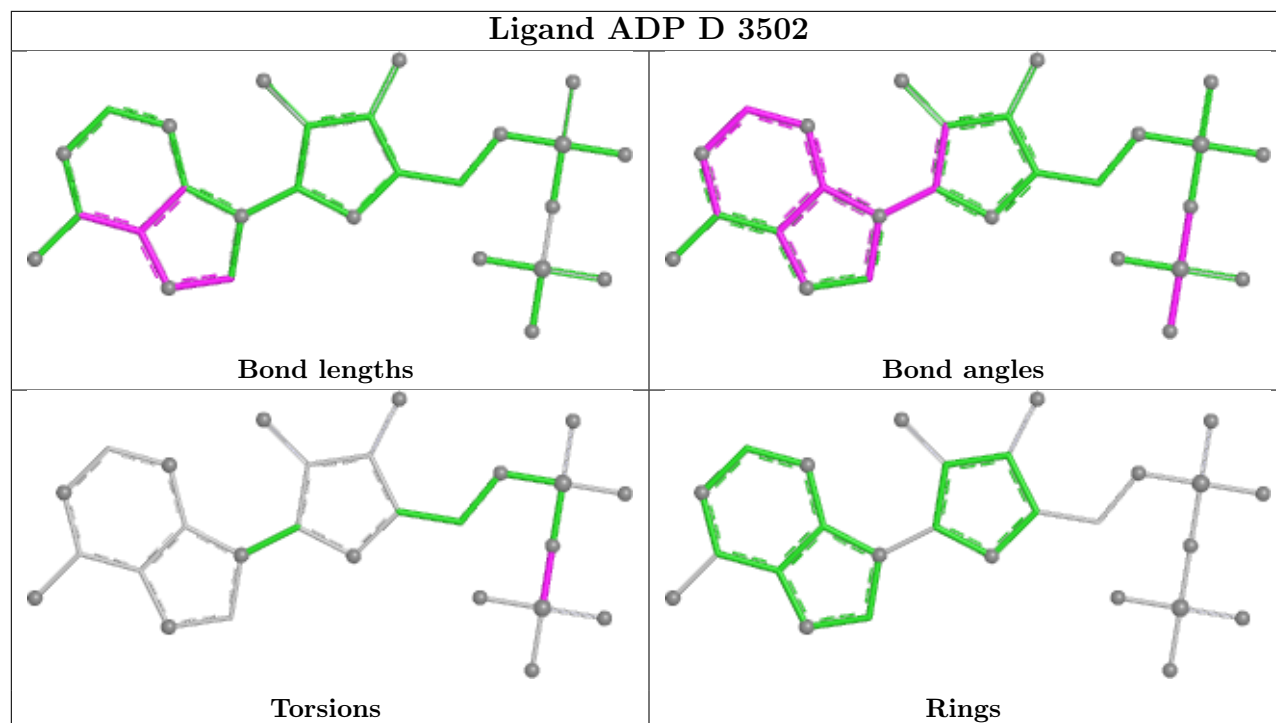
Ligand ADP A 2502

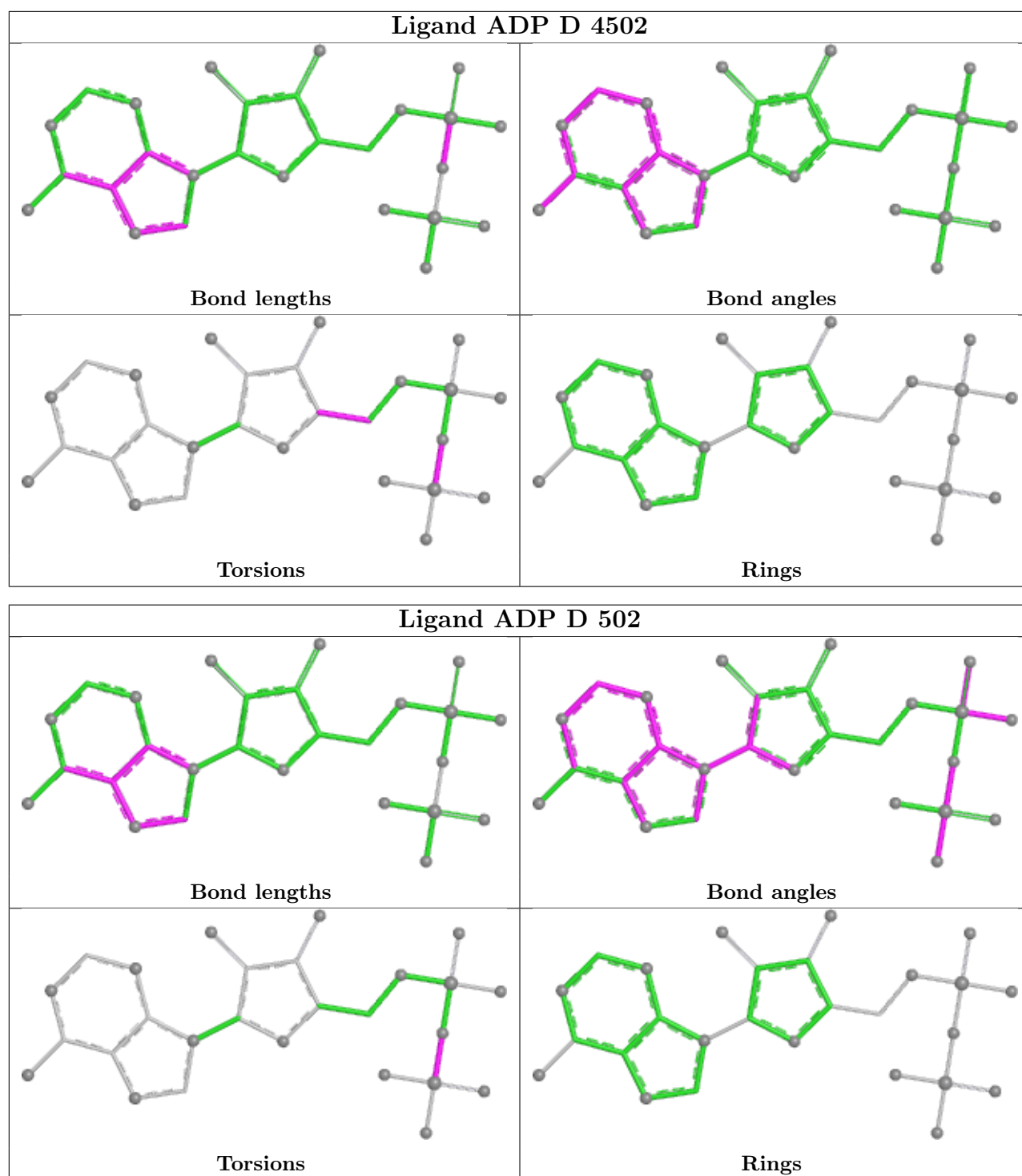


Ligand ADP A 3502









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 ⓘ

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(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

All (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
3	D	4314	GLU	3.2
3	D	4278	GLY	2.8
3	D	4319	ILE	2.8
3	D	4136	GLY	2.7
3	A	62	VAL	2.7
3	D	2236	ASN	2.7
3	D	4284	ILE	2.6
3	A	190	ILE	2.5
3	A	50	ALA	2.5
3	A	252	ALA	2.4
3	A	282	LYS	2.4
2	C	2014	DA	2.4
3	A	1289	ALA	2.4
3	D	4315	THR	2.4

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Mol	Chain	Res	Type	RSRZ
3	D	4279	VAL	2.4
3	A	4055	GLY	2.4
3	A	149	LEU	2.3
3	A	53	ALA	2.3
3	A	191	PHE	2.3
3	D	4270	PHE	2.3
3	A	251	ILE	2.2
3	A	1204	GLY	2.2
3	D	4301	GLY	2.2
3	A	142	VAL	2.1
3	D	4306	THR	2.1
3	A	212	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
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

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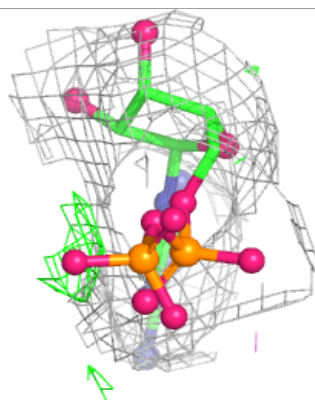
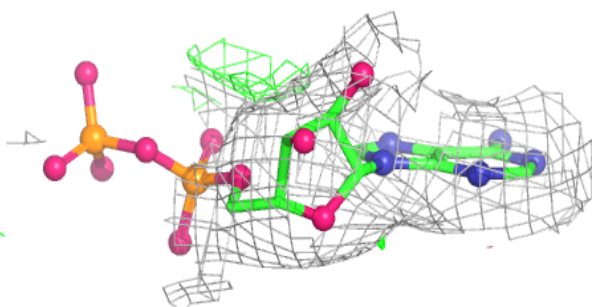
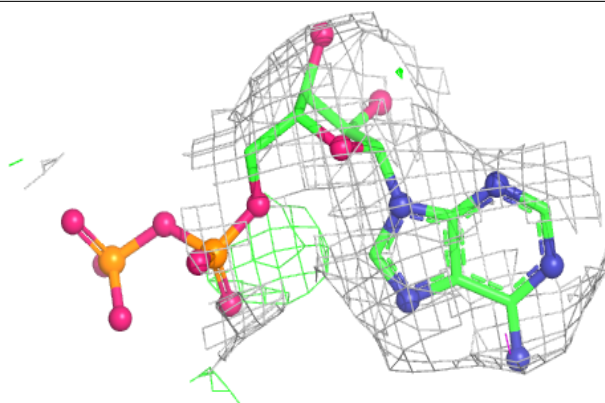
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	ALF	D	3501	5/5	0.97	0.05	2,2,3,6	0
5	ALF	A	1501	5/5	0.97	0.08	2,2,4,5	0
4	MG	D	500	1/1	0.97	0.05	5,5,5,5	0
6	ADP	A	1502	27/27	0.97	0.06	2,2,3,5	0
6	ADP	A	2502	27/27	0.97	0.06	2,2,2,5	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

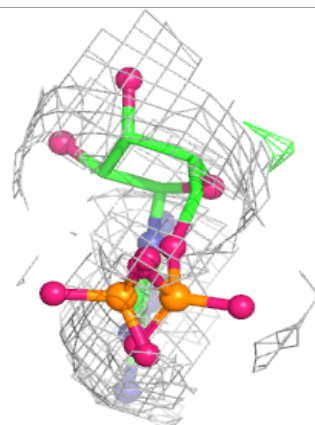
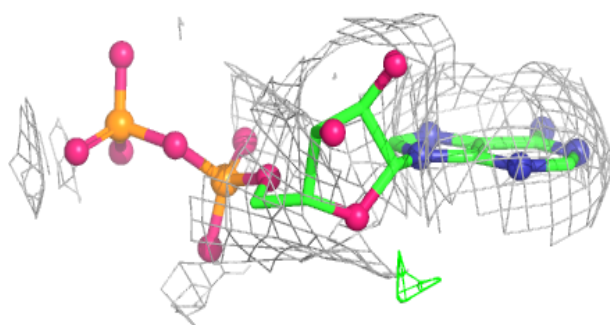
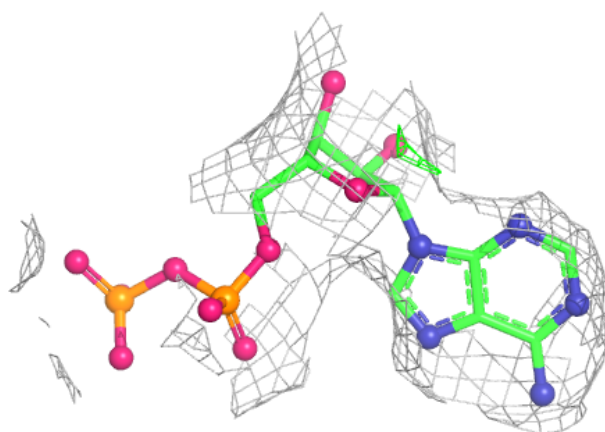
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

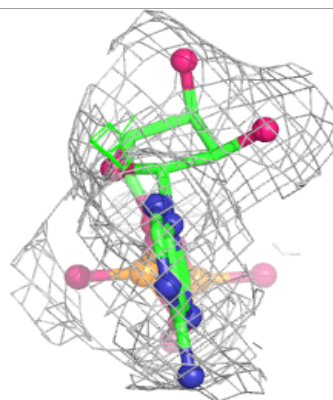
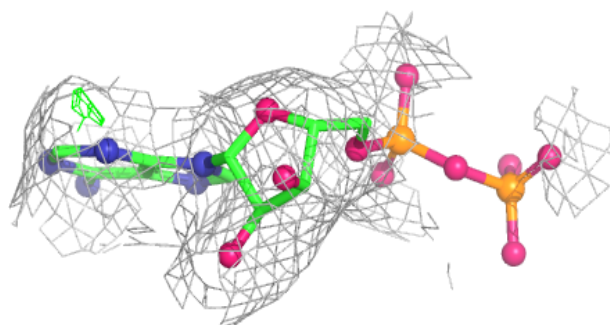
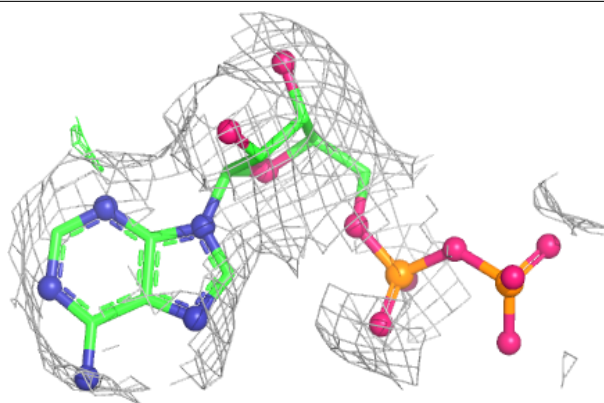
**Electron density around ADP A 4502:**

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

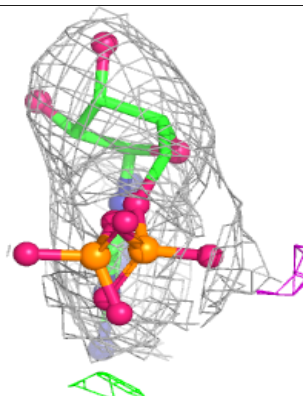
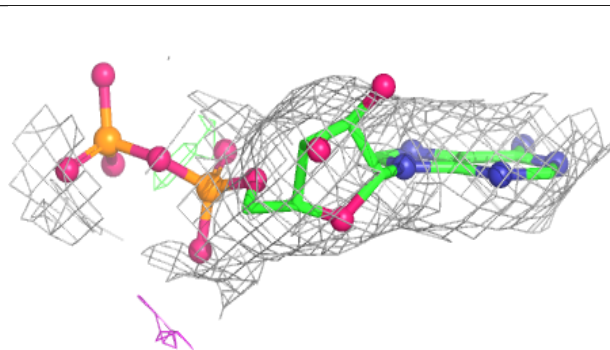
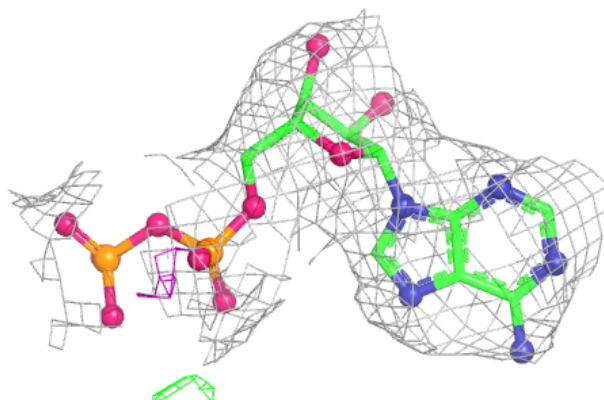


Electron density around ADP A 1502:

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

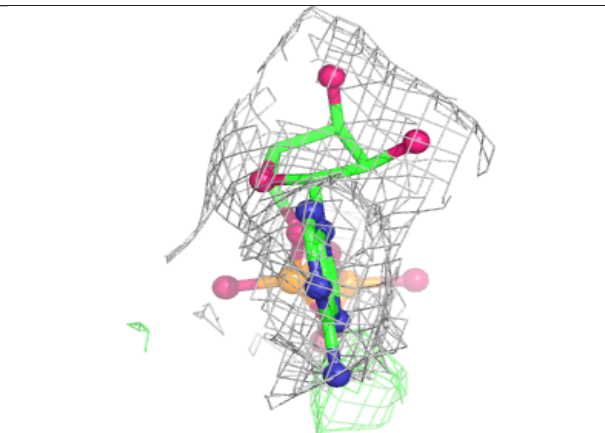
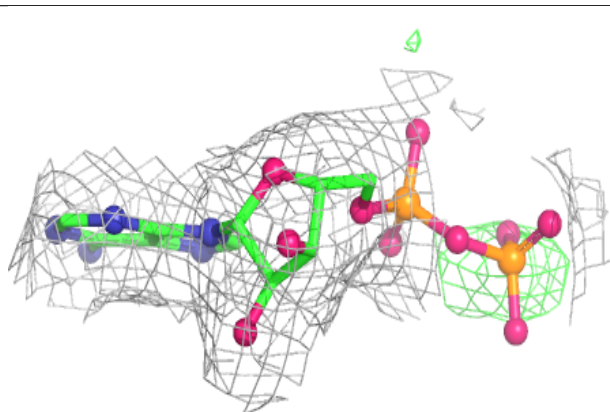
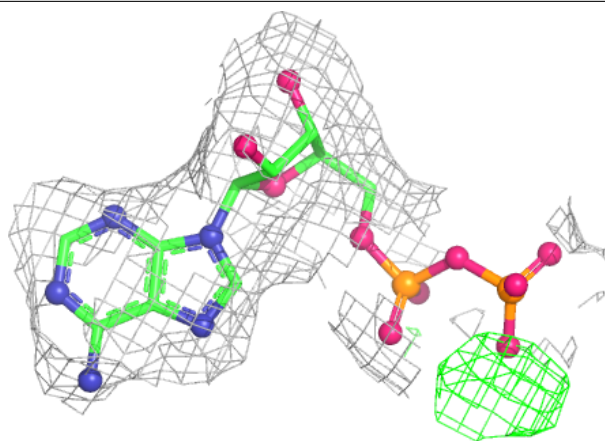
**Electron density around ADP A 2502:**

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

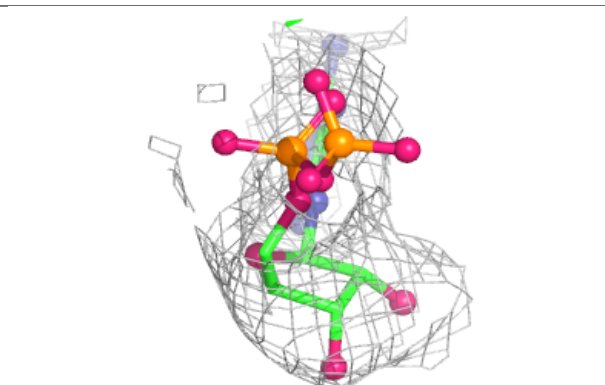
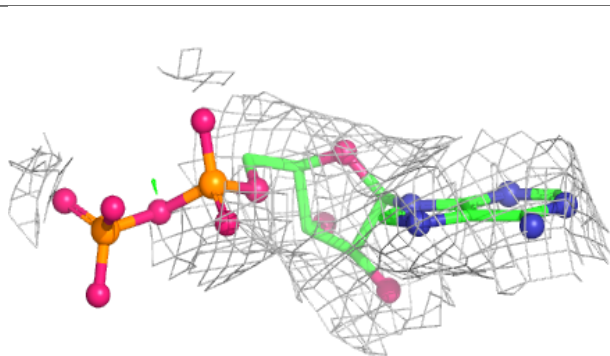
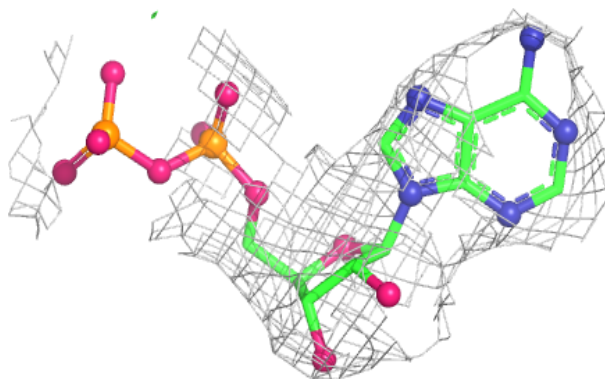


Electron density around ADP A 3502:

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

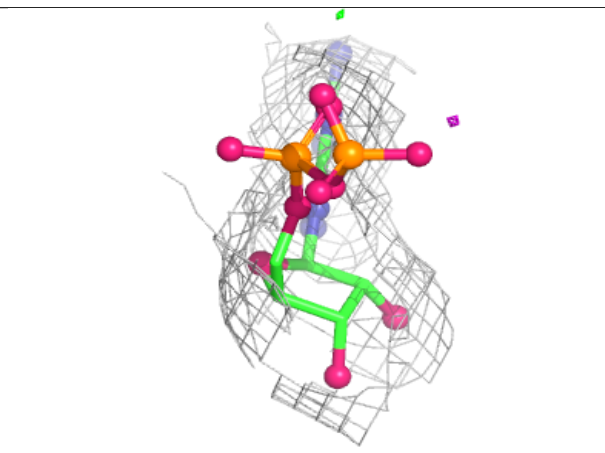
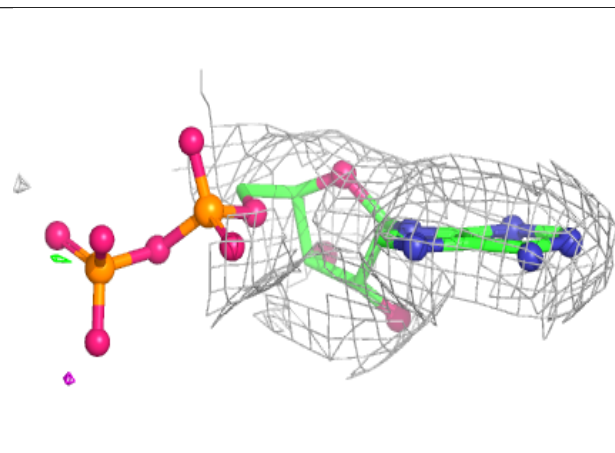
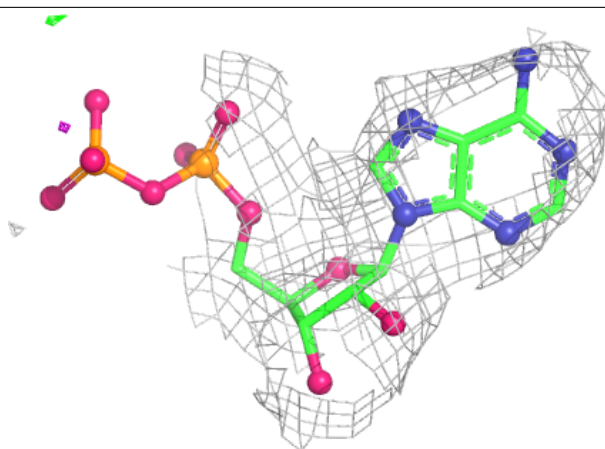
**Electron density around ADP D 3502:**

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

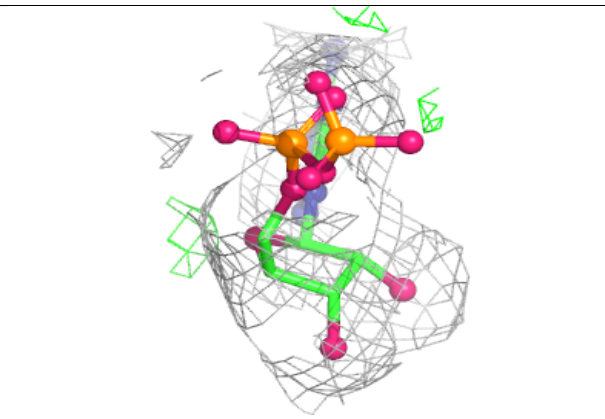
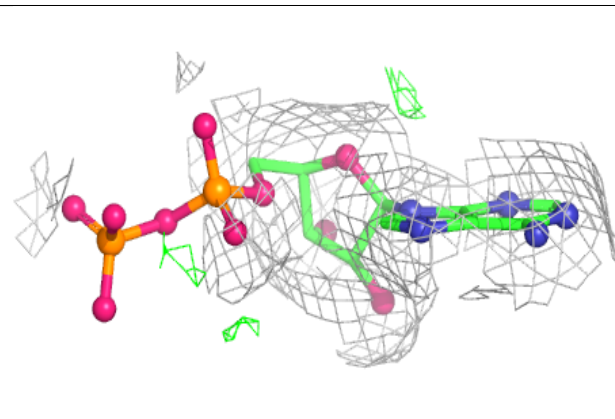
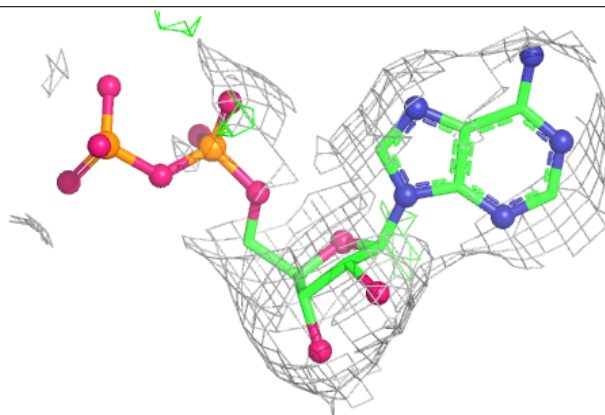


Electron density around ADP D 4502:

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

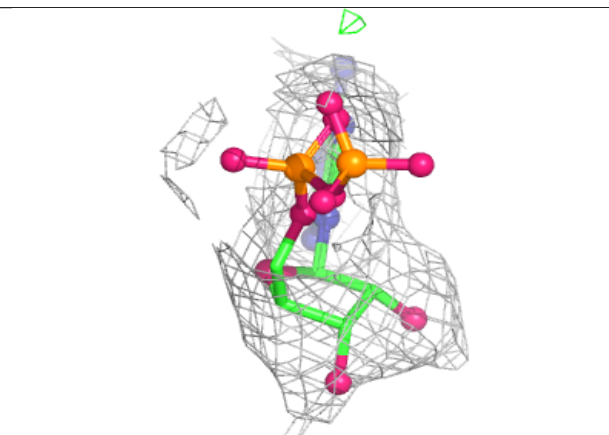
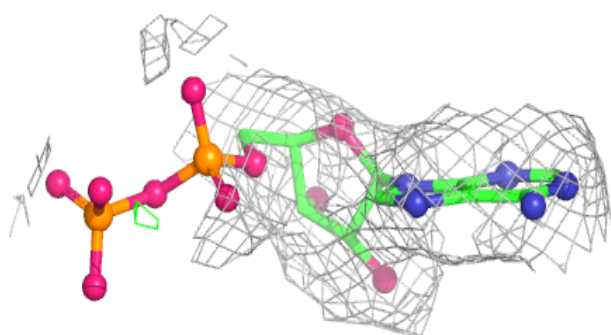
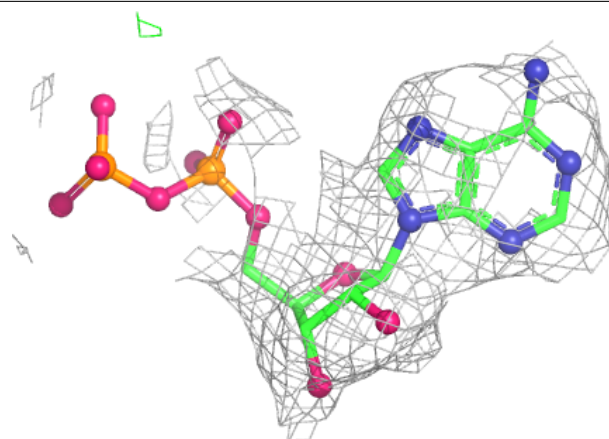
**Electron density around ADP D 1502:**

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

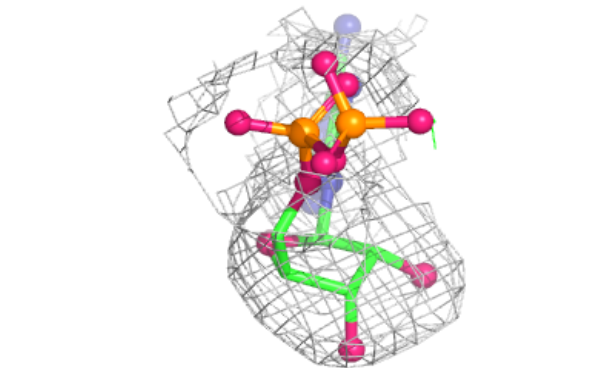
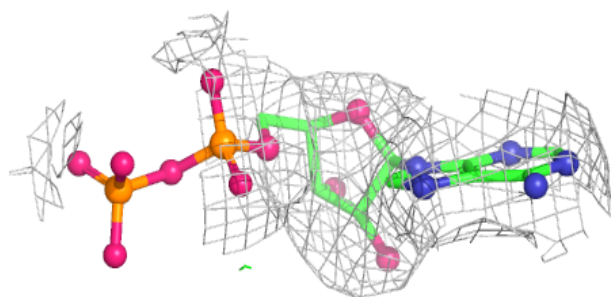
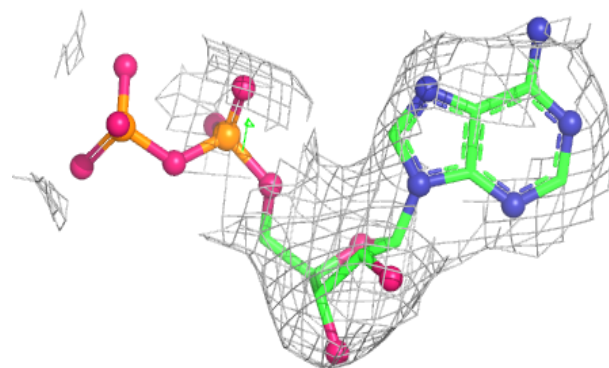


Electron density around ADP D 2502:

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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.