Full wwPDB X-ray Structure Validation Report (i)

Aug 5, 2026 – 10:20 AM EDT

PDB ID	:	3CMT / pdb_00003cmt
Title	:	Mechanism of homologous recombination from the RecA-ssDNA/dsDNA structures
Authors	:	Chen, Z.; Yang, H.; Pavletich, N.P.
Deposited on	:	2008-03-24
Resolution	:	3.15 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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

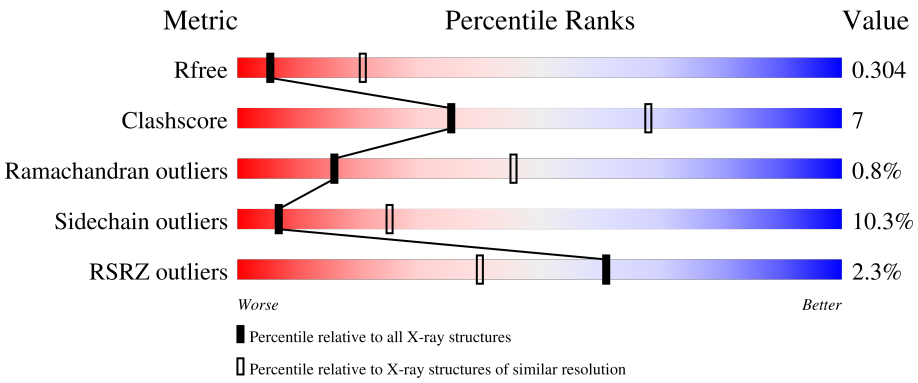
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.15 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	2361 (3.20-3.12)
Clashscore	190562	2486 (3.20-3.12)
Ramachandran outliers	187476	2405 (3.20-3.12)
Sidechain outliers	187428	2404 (3.20-3.12)
RSRZ outliers	180081	2361 (3.20-3.12)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	15	7%; 27%, 47%, 7%, 20%
1	E	15	27%, 47%, 7%, 20%
2	C	6	83%, 17%
2	F	6	83%, 17%
3	A	1706	3%; 77%, 14%, • , 6%

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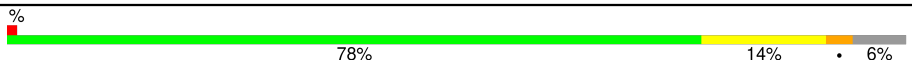
Mol	Chain	Length	Quality of chain
3	D	1706	

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 25312 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*DCP*DCP*DCP*DAP*DCP*DCP*DTP*DTP*DTP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	12	236	115	32	77	12	0	0	0
1	E	12	236	115	32	77	12	0	0	0

- Molecule 2 is a DNA chain called DNA (5'-D(P*DGP*DGP*DTP*DGP*DGP*DG)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	C	6	130	60	27	37	6	3	0	0
2	F	6	130	60	27	37	6	3	0	0

- Molecule 3 is a protein called Protein recA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	A	1609	12125	7622	2100	2347	56	0	0	0
3	D	1609	12125	7622	2101	2345	57	0	0	0

There are 130 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	linker	UNP P0A7G6
A	27	ALA	-	linker	UNP P0A7G6
A	28	MET	-	linker	UNP P0A7G6
A	29	HIS	-	linker	UNP P0A7G6
A	986	THR	-	linker	UNP P0A7G6
A	987	GLY	-	linker	UNP P0A7G6
A	988	SER	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
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
A	2999	MET	-	linker	UNP P0A7G6

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Chain	Residue	Modelled	Actual	Comment	Reference
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
D	1992	MET	-	linker	UNP P0A7G6

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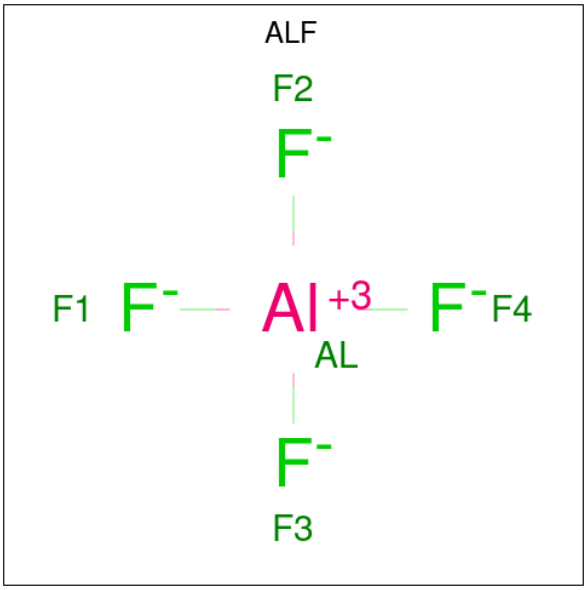
Chain	Residue	Modelled	Actual	Comment	Reference
D	1993	GLY	-	linker	UNP P0A7G6
D	1994	HIS	-	linker	UNP P0A7G6
D	1995	THR	-	linker	UNP P0A7G6
D	1996	THR	-	linker	UNP P0A7G6
D	1997	GLY	-	linker	UNP P0A7G6
D	1998	SER	-	linker	UNP P0A7G6
D	1999	MET	-	linker	UNP P0A7G6
D	2000	SER	-	linker	UNP P0A7G6
D	2985	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).

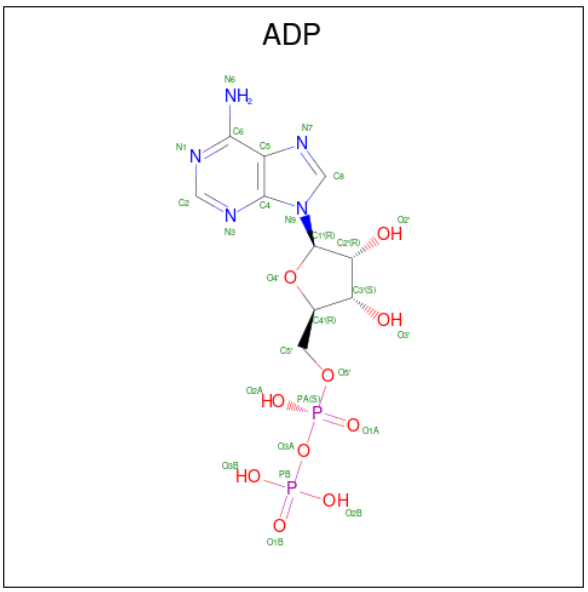
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	5	5	5	0	0
			Total	Mg		
4	D	5	5	5	0	0

- Molecule 5 is TETRAFLUOROALUMINATE ION (CCD ID: ALF) (formula: AlF_4).



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

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



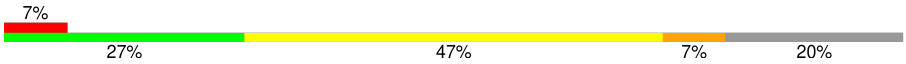
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
6	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
6	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
6	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
6	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
6	D	1	27	10	5	10	2	0	0
			Total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

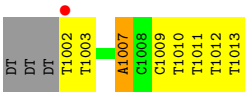
3 Residue-property plots (i)

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*DCP*DCP*DCP*DAP*DCP*DCP*DTP*DTP*DTP*DT)-3')

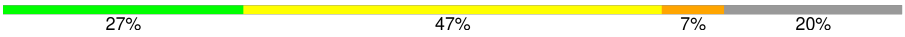
Chain B:

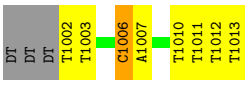




• Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DCP*DCP*DCP*DAP*DCP*DCP*DTP*DTP*DTP*DT)-3')

Chain E:





• Molecule 2: DNA (5'-D(P*DGP*DGP*DTP*DGP*DGP*DG)-3')

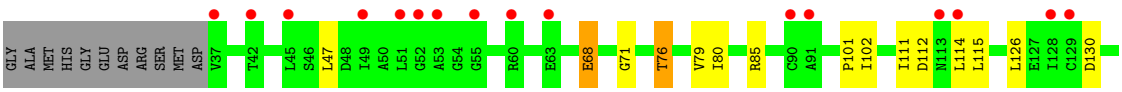
Chain C:

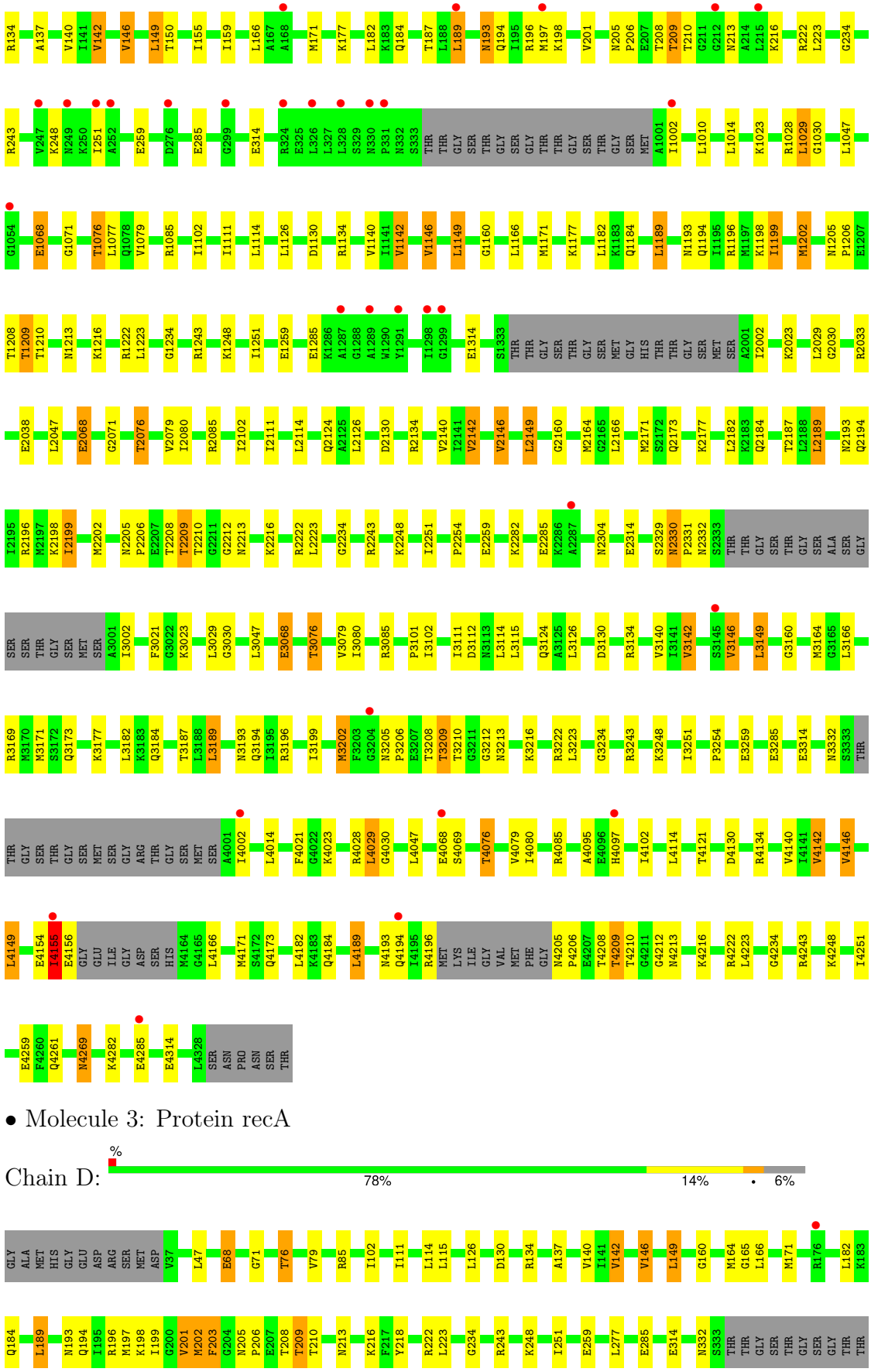
• Molecule 2: DNA (5'-D(P*DGP*DGP*DTP*DGP*DGP*DG)-3')

Chain F:

• Molecule 3: Protein recA

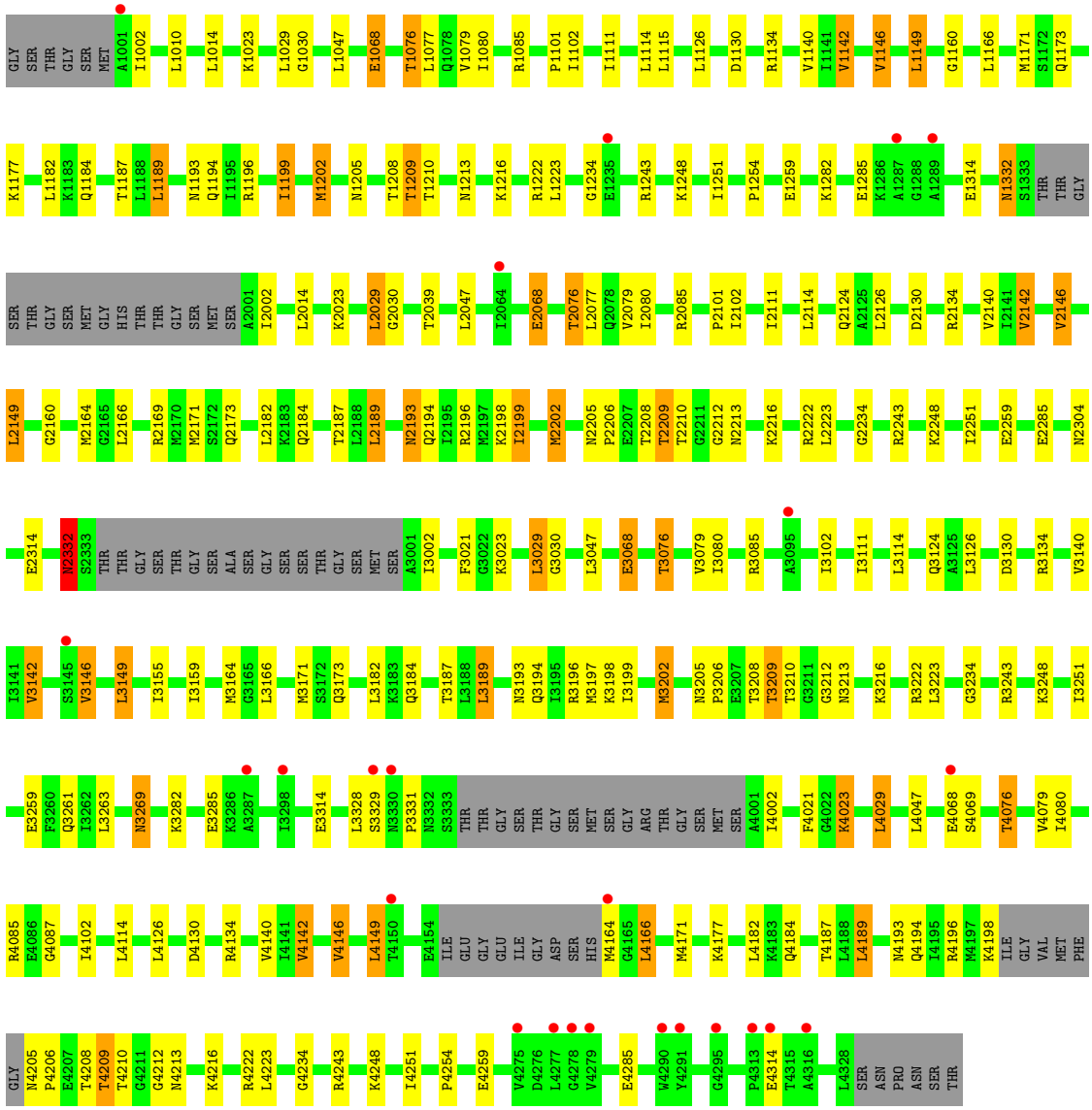
Chain A:





- Molecule 3: Protein recA

Chain D:


GLY SER THR GLY SER MET A1001 I1002 L1010 L1014 K1023 L1029 G1030 L1047 E1068 T1076 L1077 Q1078 V1079 I1080 R1085 P1101 I1102 I1111 L1114 L1115 L1126 D1130 R1134 V1140 I1141 V1142 V1146 L1149 G1160 L1166 M1171 S1172 Q1173
K1177 L1182 K1183 Q1184 T1187 L1188 L1189 N1193 Q1194 I1195 R1196 I1199 M1202 N1205 T1208 T1209 T1210 N1213 K1216 R1222 L1223 G1234 E1235 R1243 K1248 I1251 P1254 E1259 K1282 E1285 K1286 A1287 G1288 A1289 E1314 N1332 S1333 THR THR GLY
SER THR GLY SER MET GLY HIS THR THR GLY SER MET SER A2001 I2002 L2014 K2023 L2029 G2030 T2039 L2047 I2064 E2068 T2076 L2077 Q2078 V2079 I2080 R2085 P2101 I2102 I2111 L2114 Q2124 A2125 L2126 D2130 R2134 V2140 I2141 V2142 V2146
L2149 G2160 M2164 G2165 L2166 R2169 M2170 M2171 S2172 Q2173 L2182 K2183 Q2184 T2187 L2188 L2189 N2193 Q2194 I2195 R2196 M2197 K2198 I2199 M2202 N2205 P2206 E2207 T2208 T2209 T2210 G2211 G2212 N2213 K2216 R2222 L2223 G2234 R2243 K2248 I2251 E2259 E2285 N2304
E2314 N2332 S2333 THR THR GLY SER THR GLY SER ALA SER GLY SER SER THR GLY SER MET SER A3001 I3002 F3021 G3022 K3023 L3029 G3030 L3047 E3068 T3076 V3079 I3080 R3085 A3095 I3102 I3111 L3114 Q3124 A3125 L3126 D3130 R3134 V3140
I3141 V3142 S3145 V3146 L3149 I3155 I3159 M3164 G3165 L3166 M3171 S3172 Q3173 L3182 K3183 Q3184 T3187 L3188 L3189 N3193 Q3194 I3195 R3196 M3197 K3198 I3199 M3202 N3205 P3206 E3207 T3208 T3209 T3210 G3211 G3212 N3213 K3216 R3222 L3223 G3234 R3243 K3248 I3251
E3259 F3260 Q3261 I3262 L3263 N3269 K3282 E3285 K3286 A3287 I3298 E3314 L3328 S3329 N3330 P3331 N3332 S3333 THR THR GLY SER THR GLY SER MET SER GLY GLY ARG THR GLY SER MET SER A4001 I4002 F4021 G4022 K4023 L4029 L4047 E4068 S4069 T4076 V4079 I4080
R4085 E4086 G4087 I4102 L4114 L4126 D4130 R4134 V4140 I4141 V4142 V4146 L4149 T4150 E4154 ILE GLU GLY GLU ILE GLY ASP SER HIS M4164 G4165 L4166 M4171 K4177 L4182 K4183 Q4184 T4187 L4188 L4189 N4193 Q4194 I4195 R4196 M4197 K4198 ILE GLY VAL MET PHE
GLY N4205 P4206 E4207 T4208 T4209 T4210 G4211 G4212 N4213 K4216 R4222 L4223 G4234 R4243 K4248 I4251 P4254 E4259 V4275 D4276 L4277 G4278 V4279 E4285 W4290 Y4291 G4295 P4313 E4314 T4315 A4316 L4328 SER ASN PRO ASN SER THR

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	159.00Å 300.50Å 80.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.15 40.00 – 3.15	Depositor EDS
% Data completeness (in resolution range)	89.9 (40.00-3.15) 89.9 (40.00-3.15)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.10 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.3.0036	Depositor
R, R_{free}	0.217 , 0.243 0.271 , 0.304	Depositor DCC
R_{free} test set	1459 reflections (1.84%)	wwPDB-VP
Wilson B-factor (Å^2)	70.4	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 13.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	25312	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ADP, ALF

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	B	0.56	0/260	1.26	2/397 (0.5%)
1	E	0.53	0/260	1.35	2/397 (0.5%)
2	C	1.95	1/146 (0.7%)	1.28	2/225 (0.9%)
2	F	3.15	1/146 (0.7%)	2.16	1/225 (0.4%)
3	A	0.49	0/12264	0.85	0/16503
3	D	0.49	0/12264	0.85	1/16501 (0.0%)
All	All	0.56	2/25340 (0.0%)	0.88	8/34248 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	2007	DG	P-O5'	-37.85	0.84	1.60
2	C	2007	DG	P-O5'	-23.13	1.14	1.60

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	2007	DG	P-O5'-C5'	28.05	162.07	120.00
2	C	2007	DG	O5'-P-OP1	7.95	132.85	109.00
2	C	2007	DG	O5'-P-OP2	-7.27	86.18	108.00
3	D	4166	LEU	N-CA-C	-6.82	103.97	112.90
1	B	1007	DA	C5'-C4'-C3'	-6.27	105.49	114.90
1	E	1006	DC	O3'-P-O5'	-5.38	95.93	104.00
1	B	1007	DA	O3'-P-O5'	-5.38	95.93	104.00
1	E	1006	DC	C1'-O4'-C4'	-5.18	101.93	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	236	0	139	9	0
1	E	236	0	139	19	0
2	C	130	0	69	0	0
2	F	130	0	69	0	0
3	A	12125	0	12451	181	0
3	D	12125	0	12456	195	1
4	A	5	0	0	0	0
4	D	5	0	0	0	0
5	A	25	0	0	0	0
5	D	25	0	0	2	0
6	A	135	0	60	6	0
6	D	135	0	60	4	0
All	All	25312	0	25443	374	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 (374) 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:A:68:GLU:HG2	3:A:1216:LYS:HB3	1.39	1.02
3:D:68:GLU:HG2	3:D:1216:LYS:HB3	1.47	0.97
3:D:160:GLY:H	3:D:1173:GLN:HE22	1.14	0.94
3:A:2068:GLU:HG2	3:A:3216:LYS:HB3	1.54	0.87
3:D:1194:GLN:HE21	3:D:1196:ARG:HH12	1.23	0.86
3:D:4194:GLN:HE21	3:D:4196:ARG:HH12	1.23	0.86
3:D:2194:GLN:HE21	3:D:2196:ARG:HH12	1.24	0.85
3:A:194:GLN:HE21	3:A:196:ARG:HH12	1.25	0.85
3:A:3194:GLN:HE21	3:A:3196:ARG:HH12	1.25	0.85
3:D:1193:ASN:HD22	3:D:1194:GLN:H	1.25	0.84
3:A:3206:PRO:HG3	3:D:3202:MET:HB3	1.58	0.84
3:D:2193:ASN:HD22	3:D:2194:GLN:H	1.26	0.84
3:D:3068:GLU:HG2	3:D:4216:LYS:HB3	1.56	0.84
3:A:4282:LYS:HG3	3:D:1282:LYS:HG3	1.59	0.83
3:A:1194:GLN:HE21	3:A:1196:ARG:HH12	1.24	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3193:ASN:HD22	3:A:3194:GLN:H	1.26	0.83
3:A:4194:GLN:HE21	3:A:4196:ARG:HH12	1.26	0.82
3:D:1068:GLU:HG2	3:D:2216:LYS:HB3	1.61	0.82
3:D:194:GLN:HE21	3:D:196:ARG:HH12	1.25	0.82
3:A:2193:ASN:HD22	3:A:2194:GLN:H	1.27	0.81
3:A:2194:GLN:HE21	3:A:2196:ARG:HH12	1.24	0.81
3:D:3194:GLN:HE21	3:D:3196:ARG:HH12	1.26	0.81
3:A:193:ASN:HD22	3:A:194:GLN:H	1.28	0.80
3:A:1193:ASN:HD22	3:A:1194:GLN:H	1.28	0.80
3:D:160:GLY:H	3:D:1173:GLN:NE2	1.81	0.79
3:D:4193:ASN:HD22	3:D:4194:GLN:H	1.29	0.79
3:D:3193:ASN:HD22	3:D:3194:GLN:H	1.29	0.79
1:E:1002:DT:H2'	1:E:1003:DT:C6	2.19	0.78
3:D:2068:GLU:HG2	3:D:3216:LYS:HB3	1.66	0.77
3:A:1068:GLU:HG2	3:A:2216:LYS:HB3	1.66	0.77
3:D:193:ASN:HD22	3:D:194:GLN:H	1.32	0.77
1:E:1002:DT:P	3:D:165:GLY:HA2	2.25	0.77
3:A:71:GLY:HA2	6:A:502:ADP:H5'1	1.66	0.76
3:A:111:ILE:HG22	3:A:1030:GLY:CA	2.14	0.76
3:A:4193:ASN:HD22	3:A:4194:GLN:H	1.32	0.75
3:A:3068:GLU:HG2	3:A:4216:LYS:HB3	1.66	0.75
3:D:111:ILE:HG22	3:D:1030:GLY:CA	2.19	0.73
3:A:68:GLU:HG2	3:A:1216:LYS:CB	2.17	0.72
3:A:3146:VAL:HA	3:A:3149:LEU:HD22	1.77	0.67
3:D:201:VAL:HA	3:D:203:PHE:CZ	2.29	0.67
3:D:1193:ASN:HD22	3:D:1194:GLN:N	1.91	0.67
3:D:2193:ASN:HD22	3:D:2194:GLN:N	1.92	0.66
3:D:4146:VAL:HA	3:D:4149:LEU:HD22	1.77	0.66
3:D:201:VAL:HA	3:D:203:PHE:CE1	2.30	0.66
3:D:3146:VAL:HA	3:D:3149:LEU:HD22	1.78	0.66
3:A:2193:ASN:HD22	3:A:2194:GLN:N	1.94	0.65
3:D:2160:GLY:H	3:D:3173:GLN:HE22	1.41	0.65
3:D:3076:THR:HG21	3:D:3142:VAL:HG21	1.78	0.65
3:A:2068:GLU:HG2	3:A:3216:LYS:CB	2.26	0.65
3:D:146:VAL:HA	3:D:149:LEU:HD22	1.78	0.65
3:D:2160:GLY:H	3:D:3173:GLN:NE2	1.95	0.65
3:A:193:ASN:HD22	3:A:194:GLN:N	1.94	0.65
3:A:2329:SER:O	3:A:2330:ASN:HB2	1.94	0.65
3:A:4146:VAL:HA	3:A:4149:LEU:HD22	1.78	0.65
3:D:3068:GLU:HG2	3:D:4216:LYS:CB	2.27	0.65
3:D:4193:ASN:HD22	3:D:4194:GLN:N	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:112:ASP:O	3:A:1028:ARG:HG2	1.97	0.64
3:A:1193:ASN:HD22	3:A:1194:GLN:N	1.95	0.64
3:A:3193:ASN:HD22	3:A:3194:GLN:N	1.94	0.64
3:A:146:VAL:HA	3:A:149:LEU:HD22	1.79	0.64
3:A:1146:VAL:HA	3:A:1149:LEU:HD22	1.78	0.64
3:D:1111:ILE:HG22	3:D:2030:GLY:CA	2.26	0.64
3:D:3193:ASN:OD1	3:D:3209:THR:HG23	1.98	0.64
3:A:2146:VAL:HA	3:A:2149:LEU:HD22	1.80	0.64
3:D:68:GLU:HG2	3:D:1216:LYS:CB	2.26	0.64
3:A:3193:ASN:OD1	3:A:3209:THR:HG23	1.99	0.63
3:A:111:ILE:HG22	3:A:1030:GLY:N	2.13	0.63
3:A:1071:GLY:HA2	6:A:1502:ADP:H5'1	1.79	0.63
3:A:76:THR:HG21	3:A:142:VAL:HG21	1.80	0.63
3:D:193:ASN:OD1	3:D:209:THR:HG23	1.98	0.63
1:E:1013:DT:C7	3:D:3197:MET:HG3	2.29	0.63
3:A:115:LEU:HD21	3:A:1014:LEU:HD21	1.81	0.63
3:D:2146:VAL:HA	3:D:2149:LEU:HD22	1.80	0.63
1:B:1007:DA:H5'	3:A:2212:GLY:HA2	1.80	0.63
1:E:1013:DT:H71	3:D:3197:MET:HG3	1.81	0.62
3:A:1076:THR:HG21	3:A:1142:VAL:HG21	1.81	0.62
3:D:3193:ASN:HD22	3:D:3194:GLN:N	1.96	0.62
3:A:4193:ASN:HD22	3:A:4194:GLN:N	1.97	0.62
3:D:2193:ASN:OD1	3:D:2209:THR:HG23	2.00	0.62
3:A:193:ASN:OD1	3:A:209:THR:HG23	2.00	0.62
3:D:4076:THR:HG21	3:D:4142:VAL:HG21	1.82	0.62
3:D:1146:VAL:HA	3:D:1149:LEU:HD22	1.80	0.62
3:D:4193:ASN:OD1	3:D:4209:THR:HG23	1.99	0.62
3:A:4076:THR:HG21	3:A:4142:VAL:HG21	1.82	0.61
3:A:4193:ASN:OD1	3:A:4209:THR:HG23	2.00	0.61
3:D:2124:GLN:HG3	3:D:3021:PHE:CD1	2.36	0.61
3:A:2160:GLY:H	3:A:3173:GLN:NE2	1.98	0.61
3:A:3076:THR:HG21	3:A:3142:VAL:HG21	1.82	0.61
3:D:1193:ASN:OD1	3:D:1209:THR:HG23	2.00	0.61
3:A:2330:ASN:H	3:A:2331:PRO:HD3	1.65	0.60
3:A:1193:ASN:OD1	3:A:1209:THR:HG23	2.02	0.60
3:D:111:ILE:HG22	3:D:1030:GLY:HA2	1.83	0.60
1:E:1003:DT:O2	3:D:199:ILE:HG22	2.00	0.60
3:D:76:THR:HG21	3:D:142:VAL:HG21	1.84	0.60
3:A:2193:ASN:OD1	3:A:2209:THR:HG23	2.01	0.60
3:A:3111:ILE:HG22	3:A:4030:GLY:CA	2.32	0.60
3:D:1076:THR:HG21	3:D:1142:VAL:HG21	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1002:DT:H2'	1:B:1003:DT:C6	2.38	0.59
3:A:150:THR:HB	3:A:155:ILE:HD11	1.83	0.59
3:A:4121:THR:HG22	3:A:4155:ILE:HD12	1.85	0.59
3:D:193:ASN:HD22	3:D:194:GLN:N	1.98	0.59
1:E:1010:DT:H5'	3:D:3212:GLY:HA2	1.84	0.59
3:A:2160:GLY:H	3:A:3173:GLN:HE22	1.50	0.59
3:D:2076:THR:HG21	3:D:2142:VAL:HG21	1.84	0.59
3:A:2076:THR:HG21	3:A:2142:VAL:HG21	1.85	0.59
3:D:2111:ILE:HG22	3:D:3030:GLY:CA	2.33	0.58
3:D:3328:LEU:HB2	3:D:3331:PRO:HG3	1.84	0.58
3:D:3111:ILE:HG23	3:D:4029:LEU:HD13	1.86	0.58
3:D:4198:LYS:HG2	3:D:4206:PRO:O	2.03	0.58
1:E:1007:DA:H5'	3:D:2212:GLY:HA2	1.86	0.58
3:D:202:MET:O	3:D:202:MET:HG2	2.03	0.57
3:A:4213:ASN:OD1	3:A:4216:LYS:HE2	2.04	0.57
3:D:3243:ARG:NH1	3:D:3259:GLU:OE2	2.37	0.57
3:D:213:ASN:OD1	3:D:216:LYS:HE2	2.05	0.57
3:D:1243:ARG:NH1	3:D:1259:GLU:OE2	2.38	0.57
3:D:2243:ARG:NH1	3:D:2259:GLU:OE2	2.38	0.57
3:D:1194:GLN:NE2	3:D:1196:ARG:HH12	1.99	0.57
3:A:1243:ARG:NH1	3:A:1259:GLU:OE2	2.38	0.56
1:E:1013:DT:H5'	3:D:4212:GLY:HA2	1.86	0.56
3:A:2329:SER:O	3:A:2330:ASN:CB	2.53	0.56
3:A:198:LYS:HG2	3:A:206:PRO:O	2.05	0.56
3:A:2213:ASN:OD1	3:A:2216:LYS:HE2	2.05	0.56
3:D:1160:GLY:H	3:D:2173:GLN:NE2	2.03	0.56
3:D:3213:ASN:OD1	3:D:3216:LYS:HE2	2.05	0.56
3:D:2213:ASN:OD1	3:D:2216:LYS:HE2	2.05	0.56
3:D:3222:ARG:HG3	3:D:3248:LYS:HB3	1.87	0.56
3:D:1213:ASN:OD1	3:D:1216:LYS:HE2	2.05	0.56
3:A:4243:ARG:NH1	3:A:4259:GLU:OE2	2.39	0.56
3:D:3076:THR:CG2	3:D:3142:VAL:HG21	2.35	0.56
3:D:4213:ASN:OD1	3:D:4216:LYS:HE2	2.05	0.56
3:A:2194:GLN:NE2	3:A:2196:ARG:HH12	2.01	0.55
3:A:3222:ARG:HG3	3:A:3248:LYS:HB3	1.88	0.55
3:A:2304:ASN:ND2	3:D:2304:ASN:OD1	2.27	0.55
3:A:76:THR:CG2	3:A:142:VAL:HG21	2.37	0.55
3:A:3243:ARG:NH1	3:A:3259:GLU:OE2	2.39	0.55
3:D:2222:ARG:HG3	3:D:2248:LYS:HB3	1.89	0.55
1:E:1013:DT:H5"	3:D:4213:ASN:ND2	2.21	0.55
3:A:3076:THR:CG2	3:A:3142:VAL:HG21	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3213:ASN:OD1	3:A:3216:LYS:HE2	2.07	0.55
3:D:1076:THR:CG2	3:D:1142:VAL:HG21	2.37	0.55
3:A:243:ARG:NH1	3:A:259:GLU:OE2	2.40	0.54
3:A:1111:ILE:HG22	3:A:2030:GLY:CA	2.37	0.54
3:D:4243:ARG:NH1	3:D:4259:GLU:OE2	2.41	0.54
1:E:1010:DT:C2	3:D:2199:ILE:HD12	2.43	0.54
3:A:4076:THR:CG2	3:A:4142:VAL:HG21	2.38	0.54
3:A:4261:GLN:HB2	3:A:4269:ASN:HB3	1.89	0.54
3:D:1160:GLY:H	3:D:2173:GLN:HE22	1.56	0.54
3:D:4194:GLN:NE2	3:D:4196:ARG:HH12	2.00	0.54
3:A:1076:THR:CG2	3:A:1142:VAL:HG21	2.37	0.54
3:D:4076:THR:CG2	3:D:4142:VAL:HG21	2.38	0.54
3:A:213:ASN:OD1	3:A:216:LYS:HE2	2.08	0.54
3:D:222:ARG:HG3	3:D:248:LYS:HB3	1.91	0.53
3:D:243:ARG:NH1	3:D:259:GLU:OE2	2.41	0.53
3:D:1068:GLU:HG2	3:D:2216:LYS:CB	2.37	0.53
3:A:2243:ARG:NH1	3:A:2259:GLU:OE2	2.40	0.53
3:A:111:ILE:HG22	3:A:1030:GLY:HA2	1.89	0.53
3:A:1160:GLY:H	3:A:2173:GLN:NE2	2.06	0.53
3:A:4206:PRO:HG3	3:D:2202:MET:HB3	1.90	0.53
3:D:4222:ARG:HG3	3:D:4248:LYS:HB3	1.89	0.53
3:A:1222:ARG:HG3	3:A:1248:LYS:HB3	1.90	0.53
3:A:222:ARG:HG3	3:A:248:LYS:HB3	1.90	0.53
3:A:1213:ASN:OD1	3:A:1216:LYS:HE2	2.07	0.53
3:D:2076:THR:CG2	3:D:2142:VAL:HG21	2.38	0.53
3:A:194:GLN:NE2	3:A:196:ARG:HH12	2.01	0.53
3:A:4222:ARG:HG3	3:A:4248:LYS:HB3	1.90	0.52
3:D:1222:ARG:HG3	3:D:1248:LYS:HB3	1.91	0.52
3:A:3206:PRO:HG3	3:D:3202:MET:CB	2.34	0.52
3:A:4069:SER:HB3	6:A:4502:ADP:H3'	1.91	0.52
3:D:194:GLN:NE2	3:D:196:ARG:HH12	2.03	0.52
1:E:1013:DT:H73	3:D:3198:LYS:O	2.09	0.52
3:A:2222:ARG:HG3	3:A:2248:LYS:HB3	1.90	0.52
3:D:76:THR:CG2	3:D:142:VAL:HG21	2.39	0.52
3:D:1254:PRO:HG3	6:D:502:ADP:O2'	2.10	0.52
3:A:3124:GLN:HG3	3:A:4021:PHE:CD1	2.45	0.52
3:D:2194:GLN:NE2	3:D:2196:ARG:HH12	2.00	0.52
3:D:198:LYS:HG2	3:D:206:PRO:O	2.09	0.51
1:E:1007:DA:C6	3:D:1199:ILE:HG13	2.45	0.51
3:D:1194:GLN:HE22	3:D:1196:ARG:HH22	1.56	0.51
3:A:2076:THR:CG2	3:A:2142:VAL:HG21	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2194:GLN:HE22	3:A:2196:ARG:HH22	1.59	0.50
3:A:3194:GLN:NE2	3:A:3196:ARG:HH12	2.01	0.50
1:E:1003:DT:H2'	3:D:197:MET:O	2.11	0.50
3:A:2199:ILE:HD11	3:A:3164:MET:HE2	1.93	0.50
3:D:111:ILE:HG22	3:D:1030:GLY:N	2.27	0.50
3:A:101:PRO:HB3	3:A:1029:LEU:HD22	1.93	0.50
3:D:4194:GLN:HE22	3:D:4196:ARG:HH22	1.58	0.50
3:D:4069:SER:HA	6:D:4502:ADP:O3A	2.12	0.50
1:B:1009:DC:O2	3:A:3169:ARG:NH1	2.44	0.50
3:D:201:VAL:HG23	3:D:203:PHE:CD1	2.46	0.50
3:A:3160:GLY:H	3:A:4173:GLN:NE2	2.10	0.49
3:A:3194:GLN:HE22	3:A:3196:ARG:HH22	1.60	0.49
3:D:194:GLN:HE22	3:D:196:ARG:HH22	1.58	0.49
3:D:2068:GLU:HG2	3:D:3216:LYS:CB	2.40	0.49
3:A:194:GLN:HE22	3:A:196:ARG:HH22	1.59	0.49
3:A:1194:GLN:NE2	3:A:1196:ARG:HH12	2.00	0.49
3:D:2194:GLN:HE22	3:D:2196:ARG:HH22	1.58	0.49
1:B:1010:DT:H2'	1:B:1011:DT:C6	2.47	0.49
3:A:4154:GLU:C	3:A:4156:GLU:H	2.19	0.49
3:D:1182:LEU:HD11	3:D:1189:LEU:HD12	1.95	0.49
3:D:1194:GLN:HE21	3:D:1196:ARG:NH1	2.03	0.49
3:A:3111:ILE:HG22	3:A:4030:GLY:N	2.27	0.49
3:D:2101:PRO:HB3	3:D:3029:LEU:HD22	1.95	0.49
3:A:2124:GLN:HG3	3:A:3021:PHE:CD1	2.48	0.49
3:D:3261:GLN:HB2	3:D:3269:ASN:HB3	1.95	0.48
3:D:3194:GLN:HE22	3:D:3196:ARG:HH22	1.61	0.48
3:A:1194:GLN:HE22	3:A:1196:ARG:HH22	1.59	0.48
3:A:1160:GLY:H	3:A:2173:GLN:HE22	1.62	0.48
3:A:182:LEU:HD11	3:A:189:LEU:HD12	1.96	0.48
3:A:3254:PRO:HG3	6:A:2502:ADP:O2'	2.13	0.48
3:A:1182:LEU:HD11	3:A:1189:LEU:HD12	1.95	0.48
3:D:1115:LEU:HD21	3:D:2014:LEU:HD21	1.95	0.48
3:D:1194:GLN:NE2	3:D:1196:ARG:HH22	2.12	0.48
3:D:137:ALA:HB1	3:D:1010:LEU:HB2	1.95	0.48
3:D:182:LEU:HD11	3:D:189:LEU:HD12	1.96	0.47
3:A:3160:GLY:H	3:A:4173:GLN:HE22	1.61	0.47
3:A:4194:GLN:NE2	3:A:4196:ARG:HH12	2.04	0.47
3:D:1199:ILE:CD1	3:D:2164:MET:HE2	2.44	0.47
3:A:4282:LYS:HG3	3:D:1282:LYS:CG	2.40	0.47
3:D:1199:ILE:HD11	3:D:2164:MET:HE2	1.95	0.47
3:D:115:LEU:HD21	3:D:1014:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2194:GLN:NE2	3:D:2196:ARG:HH22	2.13	0.47
3:D:4194:GLN:NE2	3:D:4196:ARG:HH22	2.13	0.47
3:A:111:ILE:CG2	3:A:1030:GLY:HA2	2.44	0.47
3:A:4194:GLN:HE22	3:A:4196:ARG:HH22	1.61	0.47
3:D:194:GLN:NE2	3:D:196:ARG:HH22	2.11	0.47
3:A:2038:GLU:HA	3:A:2332:ASN:HD21	1.80	0.47
3:D:2182:LEU:HD11	3:D:2189:LEU:HD12	1.96	0.47
3:A:4182:LEU:HD11	3:A:4189:LEU:HD12	1.95	0.47
3:D:2111:ILE:HG22	3:D:3030:GLY:N	2.30	0.47
3:D:2130:ASP:OD2	3:D:2134:ARG:NH1	2.47	0.47
1:B:1011:DT:H2'	1:B:1012:DT:C6	2.50	0.46
3:A:3068:GLU:HG2	3:A:4216:LYS:CB	2.40	0.46
3:D:1068:GLU:HA	5:D:1501:ALF:F1	2.05	0.46
3:D:3182:LEU:HD11	3:D:3189:LEU:HD12	1.97	0.46
1:E:1011:DT:H2'	1:E:1012:DT:C6	2.50	0.46
3:A:2194:GLN:HE21	3:A:2196:ARG:NH1	2.04	0.46
3:D:3194:GLN:NE2	3:D:3196:ARG:HH12	2.02	0.46
3:D:4182:LEU:HD11	3:D:4189:LEU:HD12	1.97	0.46
3:A:3112:ASP:O	3:A:4028:ARG:HG2	2.16	0.46
3:A:2199:ILE:CD1	3:A:3164:MET:HE2	2.45	0.46
3:A:3111:ILE:HG23	3:A:4029:LEU:HD13	1.98	0.46
1:E:1006:DC:H5'	3:D:2169:ARG:HA	1.97	0.46
3:A:3111:ILE:HG22	3:A:4030:GLY:HA2	1.98	0.46
1:B:1010:DT:C2	3:A:2199:ILE:HD12	2.51	0.45
3:A:194:GLN:NE2	3:A:196:ARG:HH22	2.13	0.45
3:A:2194:GLN:NE2	3:A:2196:ARG:HH22	2.14	0.45
3:A:3080:ILE:HD11	3:A:3142:VAL:CG1	2.46	0.45
3:A:2126:LEU:HD21	3:A:2171:MET:HE1	1.99	0.45
3:D:1111:ILE:HG22	3:D:2030:GLY:HA2	1.96	0.45
3:A:111:ILE:HG23	3:A:1029:LEU:HB3	1.98	0.45
3:A:3126:LEU:HD21	3:A:3171:MET:HE1	1.98	0.45
3:D:1111:ILE:HG22	3:D:2030:GLY:N	2.31	0.45
1:E:1013:DT:H72	3:D:3197:MET:HG3	1.99	0.45
3:A:159:ILE:HG12	3:A:1177:LYS:HD3	1.98	0.45
3:A:2149:LEU:HD23	3:A:2171:MET:HE3	1.99	0.45
3:D:111:ILE:CG2	3:D:1030:GLY:HA2	2.47	0.45
1:B:1013:DT:H5'	3:A:4212:GLY:HA2	1.97	0.45
3:D:3263:LEU:HG	3:D:3269:ASN:HB2	1.99	0.45
3:A:2111:ILE:HG22	3:A:3030:GLY:CA	2.46	0.45
3:A:2182:LEU:HD11	3:A:2189:LEU:HD12	1.99	0.45
3:A:2130:ASP:OD2	3:A:2134:ARG:NH1	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:4177:LYS:HB3	3:D:4177:LYS:HE2	1.82	0.45
3:D:149:LEU:HD23	3:D:171:MET:CE	2.47	0.45
1:E:1013:DT:H71	3:D:3197:MET:CG	2.45	0.44
3:A:1194:GLN:NE2	3:A:1196:ARG:HH22	2.14	0.44
3:A:4194:GLN:NE2	3:A:4196:ARG:HH22	2.14	0.44
3:A:2149:LEU:HD23	3:A:2171:MET:CE	2.47	0.44
3:D:130:ASP:OD2	3:D:134:ARG:NH1	2.50	0.44
3:D:2149:LEU:HD23	3:D:2171:MET:CE	2.48	0.44
3:A:1130:ASP:OD2	3:A:1134:ARG:NH1	2.51	0.44
3:A:3182:LEU:HD11	3:A:3189:LEU:HD12	1.99	0.44
1:E:1007:DA:C5'	3:D:2212:GLY:HA2	2.47	0.44
3:D:194:GLN:HE21	3:D:196:ARG:NH1	2.05	0.43
3:D:1080:ILE:HD11	3:D:1142:VAL:CG1	2.48	0.43
3:D:1130:ASP:OD2	3:D:1134:ARG:NH1	2.51	0.43
3:A:1111:ILE:HG22	3:A:2030:GLY:HA2	2.01	0.43
3:D:2199:ILE:HD11	3:D:3164:MET:HE2	2.00	0.43
3:D:4254:PRO:HG3	6:D:3502:ADP:O2'	2.18	0.43
3:A:126:LEU:HD21	3:A:171:MET:HE1	2.00	0.43
3:A:130:ASP:OD2	3:A:134:ARG:NH1	2.51	0.43
3:A:2177:LYS:HB3	3:A:2177:LYS:HE2	1.83	0.43
3:A:3101:PRO:HB3	3:A:4029:LEU:HD22	1.99	0.43
3:D:3130:ASP:OD2	3:D:3134:ARG:NH1	2.51	0.43
3:D:3202:MET:H	3:D:3202:MET:HG2	1.66	0.43
3:A:2243:ARG:HG3	3:A:2259:GLU:HG2	2.00	0.43
3:A:3130:ASP:OD2	3:A:3134:ARG:NH1	2.51	0.43
3:D:1149:LEU:HD23	3:D:1171:MET:CE	2.48	0.43
3:D:3080:ILE:HD11	3:D:3142:VAL:CG1	2.48	0.43
3:D:2194:GLN:HE21	3:D:2196:ARG:NH1	2.04	0.43
3:D:3194:GLN:NE2	3:D:3196:ARG:HH22	2.16	0.43
3:D:4149:LEU:HD23	3:D:4171:MET:CE	2.48	0.43
3:A:1149:LEU:HD23	3:A:1171:MET:CE	2.48	0.43
3:A:3194:GLN:NE2	3:A:3196:ARG:HH22	2.15	0.43
3:A:4149:LEU:HD23	3:A:4171:MET:CE	2.49	0.43
3:A:3182:LEU:HD23	3:A:3187:THR:HB	2.00	0.43
3:D:126:LEU:HD21	3:D:171:MET:HE1	2.01	0.43
3:D:4126:LEU:HD21	3:D:4171:MET:HE1	2.01	0.43
3:D:2039:THR:HG23	3:D:2332:ASN:HD21	1.84	0.43
3:D:2111:ILE:HG22	3:D:3030:GLY:HA2	2.01	0.43
3:D:4194:GLN:HE21	3:D:4196:ARG:NH1	2.03	0.43
3:A:4080:ILE:HD11	3:A:4142:VAL:CG1	2.49	0.43
3:A:137:ALA:HB1	3:A:1010:LEU:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2126:LEU:HD21	3:D:2171:MET:HE1	2.00	0.42
3:D:2243:ARG:HG3	3:D:2259:GLU:HG2	2.01	0.42
3:A:1198:LYS:HG2	3:A:1206:PRO:O	2.19	0.42
3:D:2149:LEU:HD23	3:D:2171:MET:HE3	2.01	0.42
3:D:3124:GLN:HG3	3:D:4021:PHE:CD1	2.54	0.42
3:D:3198:LYS:HG2	3:D:3206:PRO:O	2.20	0.42
3:A:3202:MET:H	3:A:3202:MET:HG2	1.65	0.42
3:D:3159:ILE:HD13	3:D:4126:LEU:HB3	2.02	0.42
1:E:1013:DT:C7	3:D:3198:LYS:O	2.67	0.42
3:A:149:LEU:HD23	3:A:171:MET:CE	2.48	0.42
3:A:2071:GLY:HA2	6:A:2502:ADP:H5'1	2.02	0.42
3:D:2080:ILE:HD11	3:D:2142:VAL:CG1	2.48	0.42
3:D:4130:ASP:OD2	3:D:4134:ARG:NH1	2.52	0.42
3:A:1126:LEU:HD21	3:A:1171:MET:HE1	2.00	0.42
3:A:4095:ALA:O	3:A:4097:HIS:HD2	2.03	0.42
3:A:4130:ASP:OD2	3:A:4134:ARG:NH1	2.53	0.42
3:A:1243:ARG:HG3	3:A:1259:GLU:HG2	2.02	0.42
3:D:1243:ARG:HG3	3:D:1259:GLU:HG2	2.01	0.42
3:A:2182:LEU:HD23	3:A:2187:THR:HB	2.02	0.42
3:A:1068:GLU:HG2	3:A:2216:LYS:CB	2.43	0.42
3:D:2080:ILE:HD11	3:D:2142:VAL:HG13	2.02	0.42
3:D:3194:GLN:HE21	3:D:3196:ARG:NH1	2.06	0.42
3:A:2198:LYS:HG2	3:A:2206:PRO:O	2.20	0.41
3:A:3177:LYS:HB3	3:A:3177:LYS:HE2	1.82	0.41
3:A:80:ILE:HD11	3:A:142:VAL:CG1	2.50	0.41
3:D:4023:LYS:H	3:D:4023:LYS:HG2	1.74	0.41
3:A:1149:LEU:HD23	3:A:1171:MET:HE3	2.03	0.41
3:A:3149:LEU:HD23	3:A:3171:MET:CE	2.50	0.41
3:D:71:GLY:HA2	6:D:502:ADP:H5'1	2.03	0.41
3:D:3149:LEU:HD23	3:D:3171:MET:CE	2.50	0.41
1:B:1003:DT:H2'	3:A:197:MET:O	2.20	0.41
3:A:3080:ILE:HD11	3:A:3142:VAL:HG13	2.02	0.41
3:A:243:ARG:HG3	3:A:259:GLU:HG2	2.02	0.41
3:A:1202:MET:H	3:A:1202:MET:HG2	1.64	0.41
3:D:2182:LEU:HD23	3:D:2187:THR:HB	2.01	0.41
3:D:4243:ARG:HG3	3:D:4259:GLU:HG2	2.03	0.41
3:A:3149:LEU:HD23	3:A:3171:MET:HE3	2.01	0.41
3:D:1076:THR:HG22	3:D:1077:LEU:N	2.34	0.41
3:D:3126:LEU:HD21	3:D:3171:MET:HE1	2.01	0.41
3:A:177:LYS:HB3	3:A:177:LYS:HE2	1.85	0.41
3:D:1126:LEU:HD21	3:D:1171:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:3080:ILE:HD11	3:D:3142:VAL:HG13	2.02	0.41
3:A:182:LEU:HD23	3:A:187:THR:HB	2.03	0.41
3:A:2080:ILE:HD11	3:A:2142:VAL:CG1	2.50	0.41
3:D:1080:ILE:HD11	3:D:1142:VAL:HG13	2.02	0.41
3:D:1177:LYS:HB3	3:D:1177:LYS:HE2	1.84	0.41
3:D:1202:MET:H	3:D:1202:MET:HG2	1.65	0.41
3:D:3243:ARG:HG3	3:D:3259:GLU:HG2	2.02	0.41
3:D:4080:ILE:HD11	3:D:4142:VAL:CG1	2.50	0.41
3:A:2254:PRO:HG3	6:A:1502:ADP:O2'	2.21	0.41
3:A:2330:ASN:N	3:A:2331:PRO:HD3	2.35	0.41
3:D:1182:LEU:HD23	3:D:1187:THR:HB	2.03	0.41
3:D:2076:THR:HG22	3:D:2077:LEU:N	2.36	0.41
3:D:3068:GLU:HA	5:D:3501:ALF:F1	2.11	0.41
3:D:3155:ILE:HA	3:D:4177:LYS:HE3	2.03	0.41
3:A:3243:ARG:HG3	3:A:3259:GLU:HG2	2.04	0.40
3:A:4080:ILE:HD11	3:A:4142:VAL:HG13	2.03	0.40
3:A:1076:THR:HG22	3:A:1077:LEU:N	2.36	0.40
3:A:1199:ILE:HD11	3:A:2164:MET:HE2	2.02	0.40
3:A:3115:LEU:HD21	3:A:4014:LEU:HD21	2.02	0.40
3:D:4182:LEU:HD23	3:D:4187:THR:HB	2.03	0.40
3:A:149:LEU:HD23	3:A:171:MET:HE3	2.04	0.40
3:A:2033:ARG:NE	3:A:2033:ARG:HA	2.37	0.40
3:A:2282:LYS:HG3	3:D:3282:LYS:HG3	2.01	0.40
3:D:201:VAL:HG23	3:D:203:PHE:CE1	2.57	0.40
3:D:2146:VAL:O	3:D:2149:LEU:HB2	2.22	0.40
3:D:3182:LEU:HD23	3:D:3187:THR:HB	2.03	0.40
3:A:4243:ARG:HG3	3:A:4259:GLU:HG2	2.02	0.40
3:D:1101:PRO:HB3	3:D:2029:LEU:HD22	2.04	0.40
1:B:1010:DT:H5'	3:A:3212:GLY:HA2	2.04	0.40
3:D:2198:LYS:HG2	3:D:2206:PRO:O	2.22	0.40
3:D:3149:LEU:HD23	3:D:3171:MET:HE3	2.04	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:D:218:TYR:OH	3:D:4087:GLY:O[4_456]	2.19	0.01

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	1595/1706 (94%)	1549 (97%)	33 (2%)	13 (1%)	16 46
3	D	1595/1706 (94%)	1539 (96%)	43 (3%)	13 (1%)	16 46
All	All	3190/3412 (94%)	3088 (97%)	76 (2%)	26 (1%)	16 46

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	1023	LYS
3	A	2023	LYS
3	A	2330	ASN
3	A	3023	LYS
3	A	4023	LYS
3	D	1023	LYS
3	D	2023	LYS
3	D	3023	LYS
3	D	4023	LYS
3	D	1332	ASN
3	D	3269	ASN
3	D	332	ASN
3	D	2332	ASN
3	A	234	GLY
3	A	1234	GLY
3	A	2234	GLY
3	A	3234	GLY
3	A	3332	ASN
3	A	4234	GLY
3	A	4269	ASN
3	D	234	GLY
3	D	1234	GLY
3	D	2234	GLY
3	D	3234	GLY
3	D	4234	GLY

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Mol	Chain	Res	Type
3	A	4155	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
3	A	1267/1339 (95%)	1140 (90%)	127 (10%)	7 27
3	D	1267/1339 (95%)	1133 (89%)	134 (11%)	6 24
All	All	2534/2678 (95%)	2273 (90%)	261 (10%)	7 25

All (261) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	A	47	LEU
3	A	68	GLU
3	A	76	THR
3	A	79	VAL
3	A	85	ARG
3	A	102	ILE
3	A	114	LEU
3	A	140	VAL
3	A	142	VAL
3	A	146	VAL
3	A	149	LEU
3	A	166	LEU
3	A	184	GLN
3	A	189	LEU
3	A	193	ASN
3	A	201	VAL
3	A	205	ASN
3	A	208	THR
3	A	209	THR
3	A	210	THR
3	A	223	LEU
3	A	251	ILE

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Mol	Chain	Res	Type
3	A	285	GLU
3	A	314	GLU
3	A	1002	ILE
3	A	1029	LEU
3	A	1047	LEU
3	A	1068	GLU
3	A	1076	THR
3	A	1079	VAL
3	A	1085	ARG
3	A	1102	ILE
3	A	1114	LEU
3	A	1140	VAL
3	A	1142	VAL
3	A	1146	VAL
3	A	1149	LEU
3	A	1166	LEU
3	A	1184	GLN
3	A	1189	LEU
3	A	1199	ILE
3	A	1202	MET
3	A	1205	ASN
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	1314	GLU
3	A	2002	ILE
3	A	2029	LEU
3	A	2047	LEU
3	A	2068	GLU
3	A	2076	THR
3	A	2079	VAL
3	A	2085	ARG
3	A	2102	ILE
3	A	2114	LEU
3	A	2140	VAL
3	A	2142	VAL
3	A	2146	VAL
3	A	2149	LEU
3	A	2166	LEU

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Mol	Chain	Res	Type
3	A	2184	GLN
3	A	2189	LEU
3	A	2199	ILE
3	A	2202	MET
3	A	2205	ASN
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	2314	GLU
3	A	3002	ILE
3	A	3029	LEU
3	A	3047	LEU
3	A	3068	GLU
3	A	3076	THR
3	A	3079	VAL
3	A	3085	ARG
3	A	3102	ILE
3	A	3114	LEU
3	A	3140	VAL
3	A	3142	VAL
3	A	3146	VAL
3	A	3149	LEU
3	A	3166	LEU
3	A	3184	GLN
3	A	3189	LEU
3	A	3199	ILE
3	A	3202	MET
3	A	3205	ASN
3	A	3208	THR
3	A	3209	THR
3	A	3210	THR
3	A	3223	LEU
3	A	3251	ILE
3	A	3285	GLU
3	A	3314	GLU
3	A	4002	ILE
3	A	4029	LEU
3	A	4047	LEU
3	A	4068	GLU

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Mol	Chain	Res	Type
3	A	4076	THR
3	A	4079	VAL
3	A	4085	ARG
3	A	4102	ILE
3	A	4114	LEU
3	A	4140	VAL
3	A	4142	VAL
3	A	4146	VAL
3	A	4149	LEU
3	A	4155	ILE
3	A	4166	LEU
3	A	4184	GLN
3	A	4189	LEU
3	A	4205	ASN
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	A	4314	GLU
3	D	47	LEU
3	D	68	GLU
3	D	76	THR
3	D	79	VAL
3	D	85	ARG
3	D	102	ILE
3	D	114	LEU
3	D	140	VAL
3	D	142	VAL
3	D	146	VAL
3	D	149	LEU
3	D	164	MET
3	D	166	LEU
3	D	184	GLN
3	D	189	LEU
3	D	201	VAL
3	D	202	MET
3	D	203	PHE
3	D	205	ASN
3	D	208	THR
3	D	209	THR

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Mol	Chain	Res	Type
3	D	210	THR
3	D	223	LEU
3	D	251	ILE
3	D	277	LEU
3	D	285	GLU
3	D	314	GLU
3	D	1002	ILE
3	D	1029	LEU
3	D	1047	LEU
3	D	1068	GLU
3	D	1076	THR
3	D	1079	VAL
3	D	1085	ARG
3	D	1102	ILE
3	D	1114	LEU
3	D	1140	VAL
3	D	1142	VAL
3	D	1146	VAL
3	D	1149	LEU
3	D	1166	LEU
3	D	1184	GLN
3	D	1189	LEU
3	D	1199	ILE
3	D	1202	MET
3	D	1205	ASN
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	1314	GLU
3	D	1332	ASN
3	D	2002	ILE
3	D	2029	LEU
3	D	2047	LEU
3	D	2068	GLU
3	D	2076	THR
3	D	2079	VAL
3	D	2085	ARG
3	D	2102	ILE
3	D	2114	LEU

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Mol	Chain	Res	Type
3	D	2140	VAL
3	D	2142	VAL
3	D	2146	VAL
3	D	2149	LEU
3	D	2166	LEU
3	D	2184	GLN
3	D	2189	LEU
3	D	2193	ASN
3	D	2199	ILE
3	D	2202	MET
3	D	2205	ASN
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	2314	GLU
3	D	2332	ASN
3	D	3002	ILE
3	D	3029	LEU
3	D	3047	LEU
3	D	3068	GLU
3	D	3076	THR
3	D	3079	VAL
3	D	3085	ARG
3	D	3102	ILE
3	D	3114	LEU
3	D	3140	VAL
3	D	3142	VAL
3	D	3146	VAL
3	D	3149	LEU
3	D	3166	LEU
3	D	3184	GLN
3	D	3189	LEU
3	D	3199	ILE
3	D	3202	MET
3	D	3205	ASN
3	D	3208	THR
3	D	3209	THR
3	D	3210	THR
3	D	3223	LEU

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Mol	Chain	Res	Type
3	D	3251	ILE
3	D	3285	GLU
3	D	3314	GLU
3	D	3329	SER
3	D	4002	ILE
3	D	4029	LEU
3	D	4047	LEU
3	D	4068	GLU
3	D	4076	THR
3	D	4079	VAL
3	D	4085	ARG
3	D	4102	ILE
3	D	4114	LEU
3	D	4140	VAL
3	D	4142	VAL
3	D	4146	VAL
3	D	4149	LEU
3	D	4164	MET
3	D	4166	LEU
3	D	4184	GLN
3	D	4189	LEU
3	D	4205	ASN
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	4314	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) 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	1097	HIS
3	A	1173	GLN

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Mol	Chain	Res	Type
3	A	1181	ASN
3	A	1184	GLN
3	A	1193	ASN
3	A	1194	GLN
3	A	1300	GLN
3	A	1304	ASN
3	A	2097	HIS
3	A	2173	GLN
3	A	2181	ASN
3	A	2193	ASN
3	A	2194	GLN
3	A	2257	GLN
3	A	2300	GLN
3	A	2304	ASN
3	A	2332	ASN
3	A	3097	HIS
3	A	3173	GLN
3	A	3181	ASN
3	A	3193	ASN
3	A	3194	GLN
3	A	3300	GLN
3	A	3304	ASN
3	A	3330	ASN
3	A	4020	GLN
3	A	4097	HIS
3	A	4173	GLN
3	A	4181	ASN
3	A	4184	GLN
3	A	4193	ASN
3	A	4194	GLN
3	A	4300	GLN
3	A	4304	ASN
3	D	97	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	332	ASN
3	D	1097	HIS

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Mol	Chain	Res	Type
3	D	1173	GLN
3	D	1181	ASN
3	D	1193	ASN
3	D	1194	GLN
3	D	1300	GLN
3	D	1304	ASN
3	D	1332	ASN
3	D	2097	HIS
3	D	2173	GLN
3	D	2181	ASN
3	D	2193	ASN
3	D	2194	GLN
3	D	2257	GLN
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	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	4300	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ALF	A	4501	6	4,4,4	1.40	0	-		
5	ALF	A	501	6	4,4,4	1.39	0	-		
5	ALF	D	501	6	4,4,4	1.31	0	-		
6	ADP	D	2502	4,5	28,29,29	1.62	6 (21%)	43,45,45	1.68	7 (16%)
5	ALF	D	1501	6	4,4,4	1.31	0	-		
5	ALF	D	4501	6	4,4,4	1.40	0	-		
5	ALF	A	3501	6	4,4,4	1.32	0	-		
5	ALF	A	1501	6	4,4,4	1.31	0	-		
6	ADP	D	502	4,5	28,29,29	1.48	6 (21%)	43,45,45	1.78	10 (23%)
6	ADP	A	3502	4,5	28,29,29	1.60	6 (21%)	43,45,45	1.73	10 (23%)
6	ADP	D	1502	4,5	28,29,29	1.47	6 (21%)	43,45,45	1.94	13 (30%)
6	ADP	A	4502	4,5	28,29,29	1.65	5 (17%)	43,45,45	1.77	10 (23%)
6	ADP	A	1502	4,5	28,29,29	1.46	6 (21%)	43,45,45	1.93	13 (30%)
6	ADP	D	4502	4,5	28,29,29	1.63	6 (21%)	43,45,45	1.73	9 (20%)
6	ADP	A	2502	4,5	28,29,29	1.50	6 (21%)	43,45,45	1.73	8 (18%)
5	ALF	A	2501	6	4,4,4	1.34	0	-		
5	ALF	D	2501	6	4,4,4	1.30	0	-		
5	ALF	D	3501	6	4,4,4	1.27	0	-		
6	ADP	A	502	4,5	28,29,29	1.47	3 (10%)	43,45,45	1.82	8 (18%)
6	ADP	D	3502	4,5	28,29,29	1.52	6 (21%)	43,45,45	1.76	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	D	4502	4,5	-	3/16/32/32	0/3/3/3
6	ADP	D	502	4,5	-	3/16/32/32	0/3/3/3

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

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2502	ADP	C5-C4	5.38	1.48	1.39
6	D	4502	ADP	C5-C4	5.38	1.48	1.39
6	A	502	ADP	C5-C4	5.11	1.48	1.39
6	A	4502	ADP	C5-C4	4.99	1.48	1.39
6	D	3502	ADP	C5-C4	4.82	1.47	1.39
6	A	2502	ADP	C5-C4	4.72	1.47	1.39
6	D	502	ADP	C5-C4	4.67	1.47	1.39
6	A	3502	ADP	C5-C4	4.56	1.47	1.39
6	A	1502	ADP	C5-C4	4.52	1.47	1.39
6	A	3502	ADP	PA-O3A	4.50	1.64	1.59
6	D	1502	ADP	C5-C4	4.16	1.46	1.39
6	A	4502	ADP	PA-O3A	4.00	1.63	1.59
6	D	4502	ADP	PA-O3A	3.95	1.63	1.59
6	D	2502	ADP	PA-O3A	3.85	1.63	1.59
6	D	1502	ADP	PA-O3A	3.53	1.63	1.59
6	D	3502	ADP	PA-O3A	3.26	1.63	1.59
6	A	2502	ADP	PA-O3A	3.02	1.62	1.59
6	A	502	ADP	C5-C6	2.87	1.49	1.41
6	D	502	ADP	PA-O3A	2.85	1.62	1.59
6	D	2502	ADP	C8-N7	2.78	1.37	1.31
6	A	1502	ADP	C5-N7	-2.68	1.34	1.39
6	D	1502	ADP	C5-N7	-2.68	1.34	1.39
6	A	4502	ADP	C5-N7	-2.62	1.34	1.39
6	D	3502	ADP	C5-N7	-2.59	1.34	1.39
6	D	502	ADP	C5-N7	-2.57	1.34	1.39
6	A	3502	ADP	C5-N7	-2.52	1.34	1.39
6	D	4502	ADP	C8-N7	2.52	1.36	1.31
6	A	2502	ADP	C5-C6	2.51	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2502	ADP	C5-N7	-2.51	1.34	1.39
6	A	1502	ADP	PA-O3A	2.50	1.62	1.59
6	D	4502	ADP	C5-C6	2.50	1.47	1.41
6	A	502	ADP	C8-N7	2.50	1.36	1.31
6	A	3502	ADP	C4-N9	-2.43	1.32	1.37
6	D	502	ADP	C5-C6	2.43	1.47	1.41
6	D	502	ADP	C8-N7	2.42	1.36	1.31
6	A	4502	ADP	C8-N7	2.41	1.36	1.31
6	A	4502	ADP	C5-C6	2.36	1.47	1.41
6	A	1502	ADP	C5-C6	2.34	1.47	1.41
6	D	3502	ADP	C8-N7	2.33	1.36	1.31
6	A	2502	ADP	C4-N9	-2.31	1.32	1.37
6	D	3502	ADP	C4-N9	-2.30	1.32	1.37
6	A	1502	ADP	C4-N9	-2.28	1.33	1.37
6	D	2502	ADP	C5-C6	2.27	1.47	1.41
6	A	1502	ADP	C8-N7	2.26	1.36	1.31
6	D	1502	ADP	C8-N7	2.24	1.36	1.31
6	D	502	ADP	C4-N9	-2.22	1.33	1.37
6	A	3502	ADP	C8-N7	2.19	1.35	1.31
6	A	2502	ADP	C8-N7	2.19	1.35	1.31
6	D	3502	ADP	C5-C6	2.18	1.47	1.41
6	D	2502	ADP	C5-N7	-2.10	1.35	1.39
6	D	4502	ADP	C5-N7	-2.09	1.35	1.39
6	D	1502	ADP	C5-C6	2.09	1.46	1.41
6	D	1502	ADP	C4-N9	-2.08	1.33	1.37
6	D	2502	ADP	C4-N9	-2.07	1.33	1.37
6	A	3502	ADP	C5-C6	2.03	1.46	1.41
6	D	4502	ADP	C4-N9	-2.02	1.33	1.37

All (98) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1502	ADP	C5-C4-N3	-5.92	118.57	126.72
6	D	502	ADP	C5-C4-N3	-5.60	119.00	126.72
6	A	4502	ADP	C5-C4-N3	-5.41	119.26	126.72
6	D	3502	ADP	C5-C4-N3	-5.35	119.34	126.72
6	A	502	ADP	C5-C4-N3	-5.29	119.44	126.72
6	A	2502	ADP	C5-C4-N3	-5.16	119.61	126.72
6	A	1502	ADP	C5-C4-N3	-5.08	119.73	126.72
6	D	1502	ADP	N3-C4-N9	4.97	135.63	127.17
6	A	3502	ADP	C5-C4-N3	-4.88	120.00	126.72
6	A	1502	ADP	N3-C4-N9	4.73	135.20	127.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	502	ADP	N3-C4-N9	4.70	135.16	127.17
6	D	4502	ADP	C5-C4-N3	-4.68	120.27	126.72
6	A	4502	ADP	N3-C4-N9	4.67	135.12	127.17
6	D	3502	ADP	N3-C4-N9	4.58	134.96	127.17
6	A	3502	ADP	N3-C4-N9	4.39	134.64	127.17
6	A	2502	ADP	N3-C4-N9	4.36	134.59	127.17
6	D	2502	ADP	C5-C4-N3	-4.33	120.75	126.72
6	D	502	ADP	N3-C4-N9	4.29	134.46	127.17
6	D	4502	ADP	N3-C4-N9	4.23	134.37	127.17
6	A	1502	ADP	N3-C2-N1	-4.13	122.33	128.58
6	D	2502	ADP	N3-C4-N9	4.01	133.98	127.17
6	D	2502	ADP	N3-C2-N1	-3.83	122.78	128.58
6	A	1502	ADP	C2-N3-C4	3.77	121.04	111.83
6	A	3502	ADP	N3-C2-N1	-3.76	122.89	128.58
6	D	1502	ADP	C2-N3-C4	3.69	120.84	111.83
6	D	4502	ADP	N3-C2-N1	-3.53	123.24	128.58
6	A	502	ADP	C2-N3-C4	3.52	120.43	111.83
6	A	4502	ADP	N3-C2-N1	-3.51	123.26	128.58
6	A	1502	ADP	C4-N9-C8	3.41	109.32	105.74
6	A	4502	ADP	C2-N3-C4	3.39	120.12	111.83
6	D	1502	ADP	N3-C2-N1	-3.31	123.57	128.58
6	A	3502	ADP	C2-N3-C4	3.29	119.87	111.83
6	A	2502	ADP	C2-N3-C4	3.26	119.79	111.83
6	A	502	ADP	N3-C2-N1	-3.26	123.65	128.58
6	D	3502	ADP	C2-N3-C4	3.24	119.73	111.83
6	D	3502	ADP	C2'-C1'-N9	-3.23	105.27	113.30
6	D	502	ADP	C2-N3-C4	3.23	119.72	111.83
6	A	502	ADP	C4-N9-C8	3.23	109.12	105.74
6	D	2502	ADP	C2-N3-C4	3.22	119.69	111.83
6	D	2502	ADP	C2-N1-C6	3.22	124.01	118.73
6	D	502	ADP	C4-C5-N7	-3.20	106.92	110.58
6	D	4502	ADP	C2-N3-C4	3.13	119.48	111.83
6	D	4502	ADP	C4-N9-C8	3.04	108.93	105.74
6	D	3502	ADP	N3-C2-N1	-2.99	124.05	128.58
6	D	1502	ADP	C4-N9-C8	2.98	108.87	105.74
6	A	4502	ADP	C4-N9-C8	2.98	108.86	105.74
6	D	2502	ADP	C4-N9-C8	2.96	108.84	105.74
6	A	4502	ADP	C4-C5-N7	-2.95	107.21	110.58
6	A	2502	ADP	N3-C2-N1	-2.93	124.15	128.58
6	D	1502	ADP	C2'-C1'-N9	-2.90	106.10	113.30
6	A	3502	ADP	C4-N9-C8	2.89	108.78	105.74
6	D	1502	ADP	C4-C5-N7	-2.85	107.32	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	4502	ADP	C2-N1-C6	2.84	123.39	118.73
6	D	3502	ADP	O4'-C1'-N9	2.81	113.49	108.09
6	A	2502	ADP	C4-N9-C8	2.70	108.58	105.74
6	A	2502	ADP	C2'-C1'-N9	-2.65	106.72	113.30
6	A	502	ADP	C4-C5-N7	-2.63	107.58	110.58
6	A	1502	ADP	N6-C6-N1	2.63	124.22	118.38
6	A	2502	ADP	C4-C5-N7	-2.62	107.59	110.58
6	A	3502	ADP	C2-N1-C6	2.60	123.00	118.73
6	A	1502	ADP	C2'-C1'-N9	-2.59	106.87	113.30
6	D	502	ADP	N3-C2-N1	-2.48	124.83	128.58
6	D	2502	ADP	C2'-C1'-N9	-2.45	107.21	113.30
6	D	4502	ADP	C4-C5-N7	-2.45	107.78	110.58
6	A	1502	ADP	O2B-PB-O3A	-2.41	96.57	104.64
6	D	4502	ADP	O3B-PB-O2B	2.38	116.73	107.80
6	D	502	ADP	C2'-C1'-N9	-2.37	107.40	113.30
6	D	3502	ADP	C4-N9-C8	2.37	108.23	105.74
6	D	502	ADP	O4'-C1'-N9	2.33	112.56	108.09
6	D	1502	ADP	N6-C6-N1	2.32	123.54	118.38
6	A	4502	ADP	C2-N1-C6	2.30	122.52	118.73
6	D	502	ADP	C4-N9-C8	2.24	108.09	105.74
6	A	1502	ADP	C2-N1-C6	2.24	122.42	118.73
6	A	4502	ADP	C5-N7-C8	2.23	106.95	103.45
6	D	1502	ADP	C5-N7-C8	2.22	106.94	103.45
6	D	502	ADP	O2B-PB-O3A	-2.22	97.19	104.64
6	D	3502	ADP	C4-C5-N7	-2.17	108.10	110.58
6	A	3502	ADP	O4'-C1'-N9	2.16	112.24	108.09
6	A	3502	ADP	C2'-C1'-N9	-2.16	107.94	113.30
6	A	4502	ADP	N6-C6-N1	2.15	123.17	118.38
6	D	4502	ADP	C2'-C1'-N9	-2.15	107.96	113.30
6	D	1502	ADP	O4'-C1'-N9	2.14	112.20	108.09
6	A	502	ADP	C5-N7-C8	2.14	106.81	103.45
6	A	1502	ADP	C4-C5-N7	-2.13	108.14	110.58
6	D	502	ADP	C5-N7-C8	2.13	106.80	103.45
6	D	3502	ADP	O2B-PB-O3A	-2.13	97.51	104.64
6	A	4502	ADP	O2B-PB-O1B	2.12	119.11	110.83
6	D	1502	ADP	O2B-PB-O1B	2.12	119.09	110.83
6	A	2502	ADP	N6-C6-N1	2.11	123.07	118.38
6	A	1502	ADP	O3B-PB-O2B	2.10	115.68	107.80
6	A	1502	ADP	C5-C6-N6	-2.09	118.12	123.29
6	D	3502	ADP	C2-N1-C6	2.06	122.12	118.73
6	A	1502	ADP	N9-C8-N7	-2.04	111.04	113.94
6	A	3502	ADP	C4-C5-N7	-2.04	108.25	110.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	D	1502	ADP	C2-N1-C6	2.04	122.08	118.73
6	A	3502	ADP	O2B-PB-O3A	-2.03	97.82	104.64
6	D	1502	ADP	N9-C8-N7	-2.02	111.07	113.94
6	A	502	ADP	N9-C8-N7	-2.01	111.08	113.94

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	502	ADP	O4'-C4'-C5'-O5'
6	A	502	ADP	PA-O3A-PB-O1B
6	A	1502	ADP	PA-O3A-PB-O1B
6	A	2502	ADP	PA-O3A-PB-O1B
6	A	3502	ADP	PA-O3A-PB-O1B
6	D	502	ADP	PA-O3A-PB-O1B
6	D	2502	ADP	PA-O3A-PB-O1B
6	D	3502	ADP	PA-O3A-PB-O3B
6	A	4502	ADP	O4'-C4'-C5'-O5'
6	A	2502	ADP	C5'-O5'-PA-O1A
6	D	4502	ADP	O4'-C4'-C5'-O5'
6	A	4502	ADP	PA-O3A-PB-O1B
6	D	3502	ADP	PA-O3A-PB-O1B
6	D	4502	ADP	PA-O3A-PB-O1B
6	A	502	ADP	PA-O3A-PB-O2B
6	A	502	ADP	PA-O3A-PB-O3B
6	A	1502	ADP	PA-O3A-PB-O2B
6	A	1502	ADP	PA-O3A-PB-O3B
6	A	2502	ADP	PA-O3A-PB-O2B
6	A	2502	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-O2B
6	A	4502	ADP	PA-O3A-PB-O3B
6	D	502	ADP	PA-O3A-PB-O2B
6	D	502	ADP	PA-O3A-PB-O3B
6	D	1502	ADP	PA-O3A-PB-O2B
6	D	1502	ADP	PA-O3A-PB-O3B
6	D	2502	ADP	PA-O3A-PB-O2B
6	D	2502	ADP	PA-O3A-PB-O3B
6	D	4502	ADP	PA-O3A-PB-O3B
6	A	2502	ADP	O4'-C4'-C5'-O5'
6	A	502	ADP	C3'-C4'-C5'-O5'

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

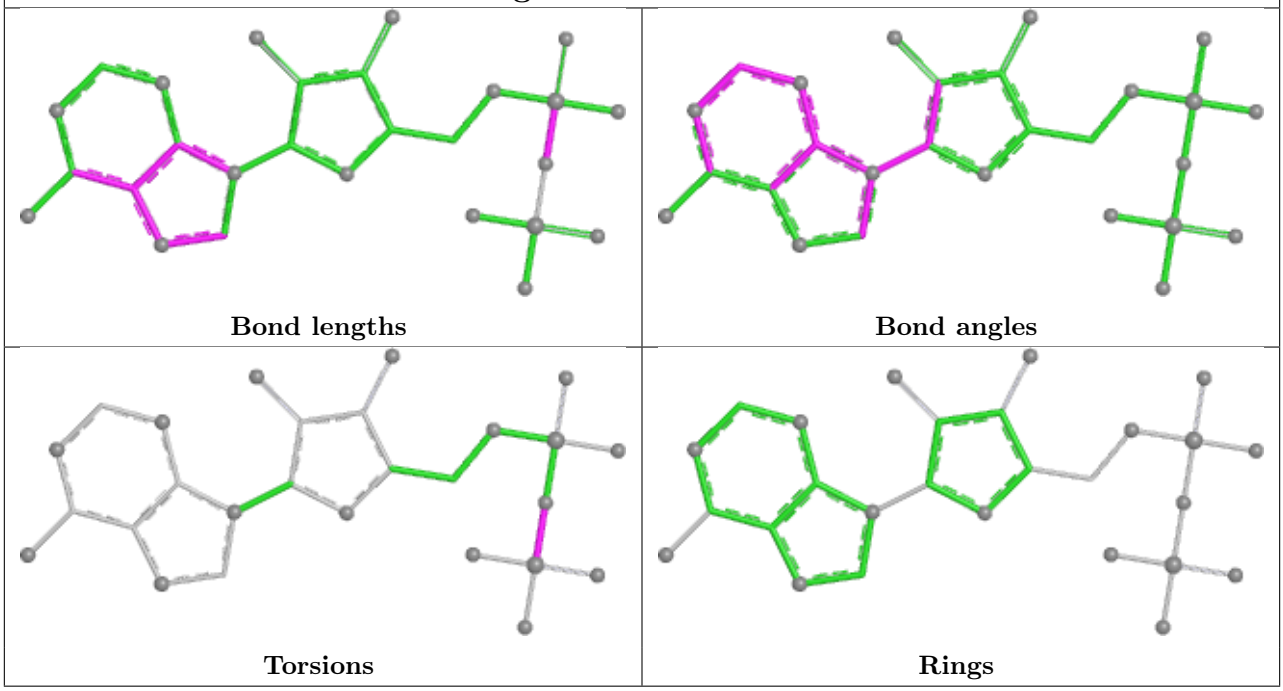
There are no ring outliers.

9 monomers are involved in 12 short contacts:

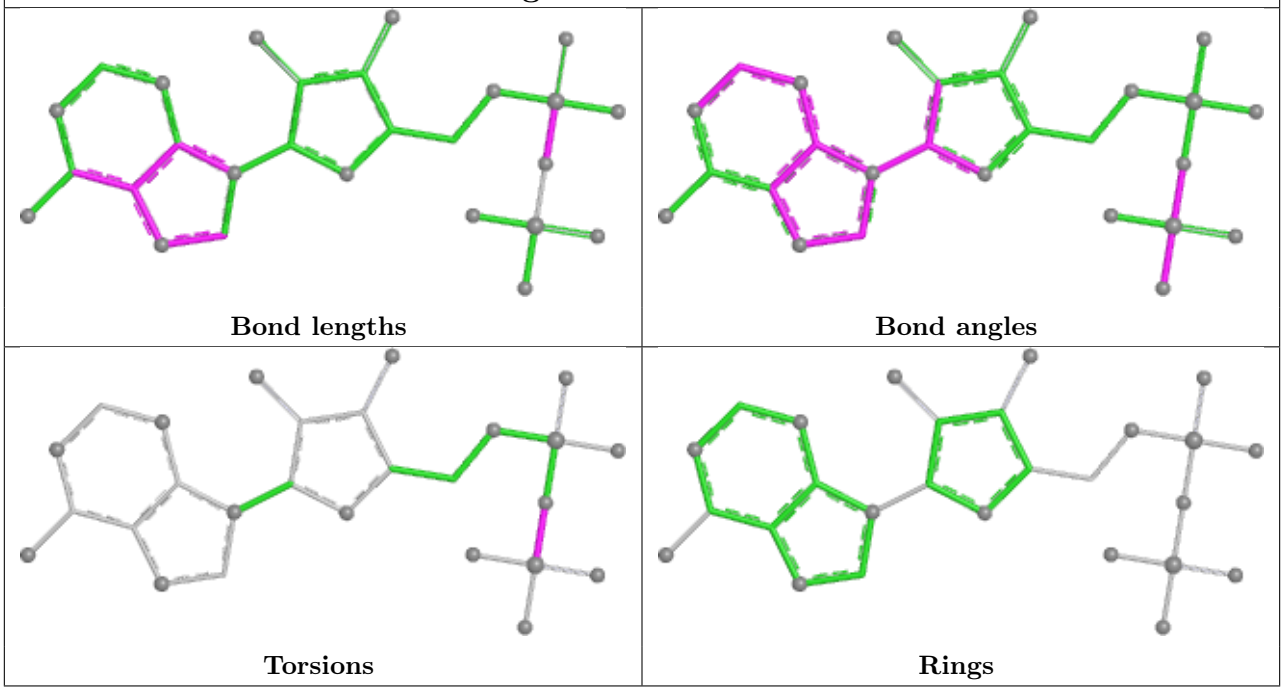
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1501	ALF	1	0
6	D	502	ADP	2	0
6	A	4502	ADP	1	0
6	A	1502	ADP	2	0
6	D	4502	ADP	1	0
6	A	2502	ADP	2	0
5	D	3501	ALF	1	0
6	A	502	ADP	1	0
6	D	3502	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

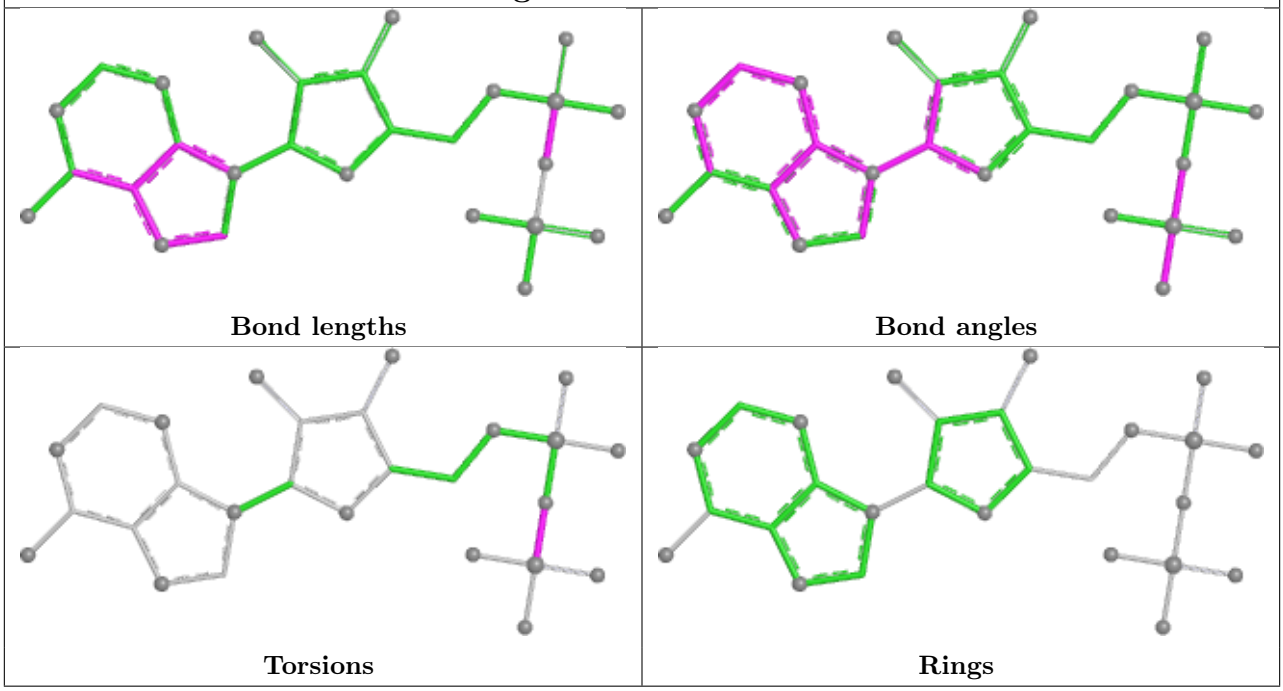
Ligand ADP D 2502



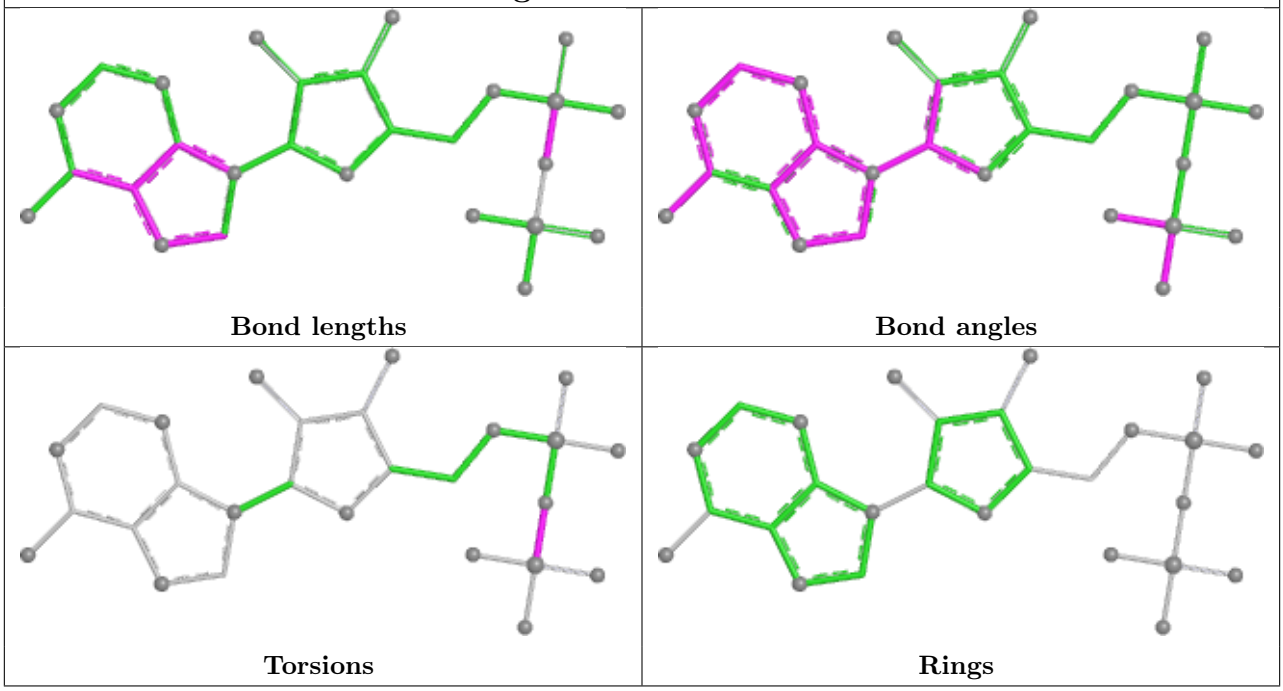
Ligand ADP D 502



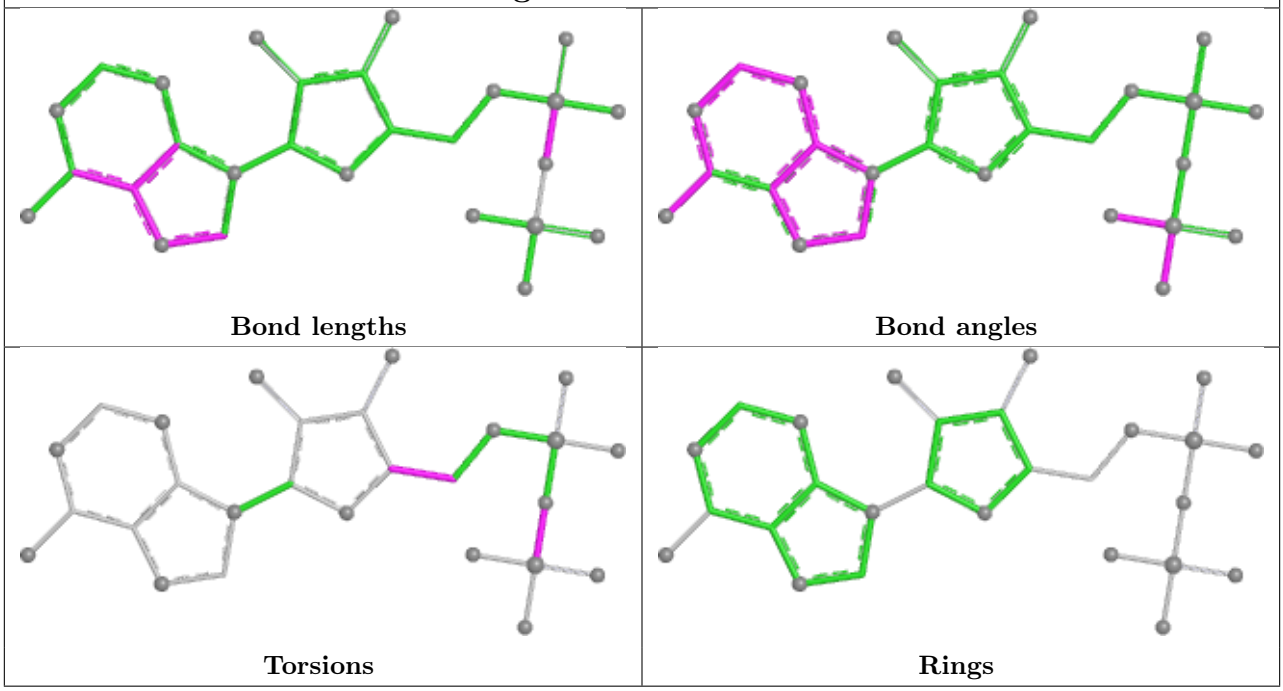
Ligand ADP A 3502



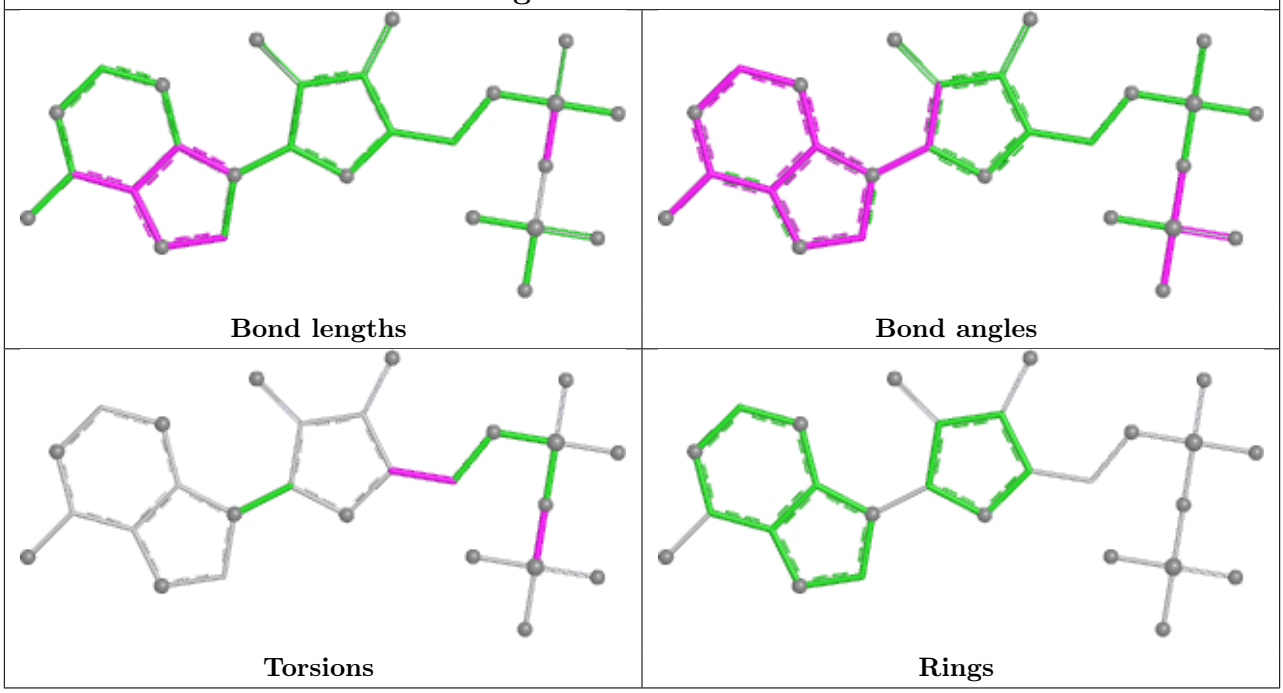
Ligand ADP D 1502



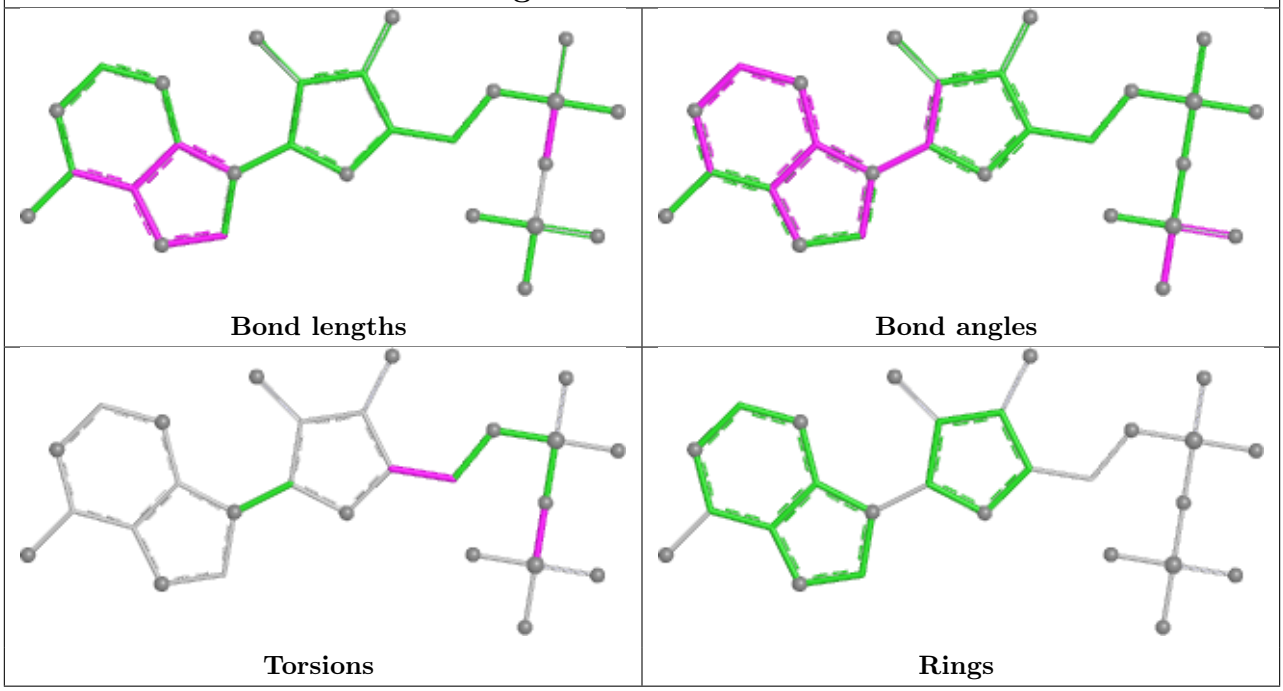
Ligand ADP A 4502



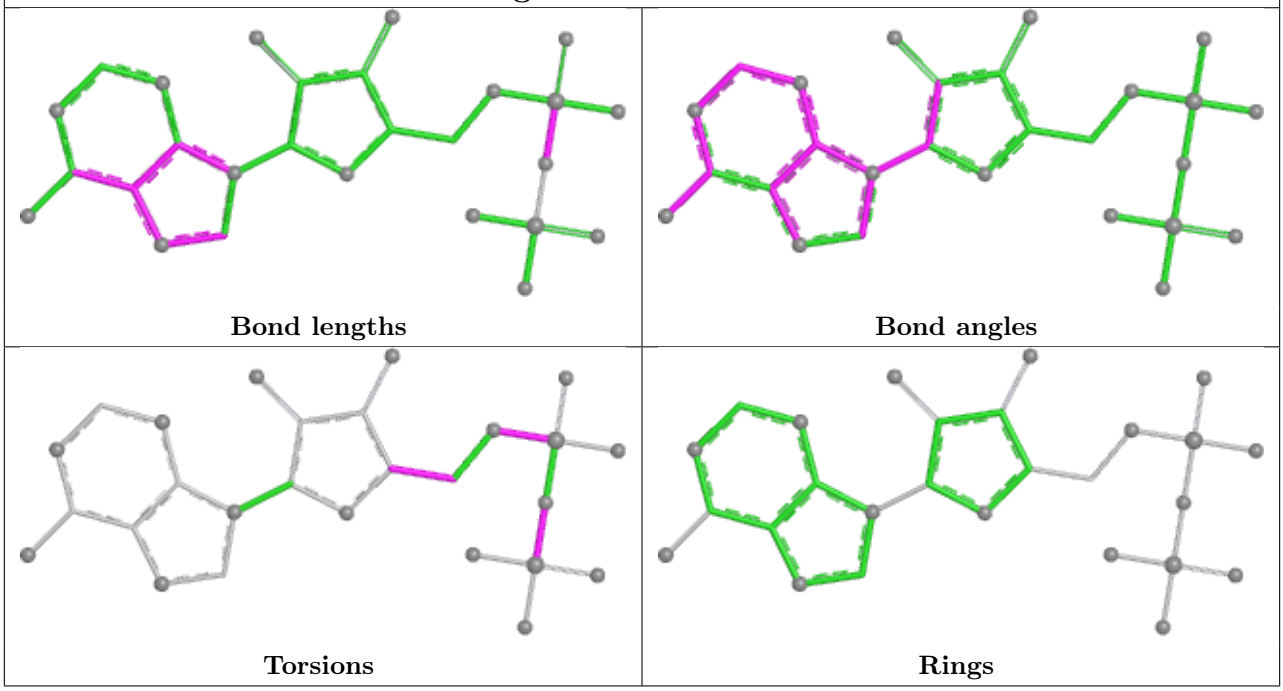
Ligand ADP A 1502



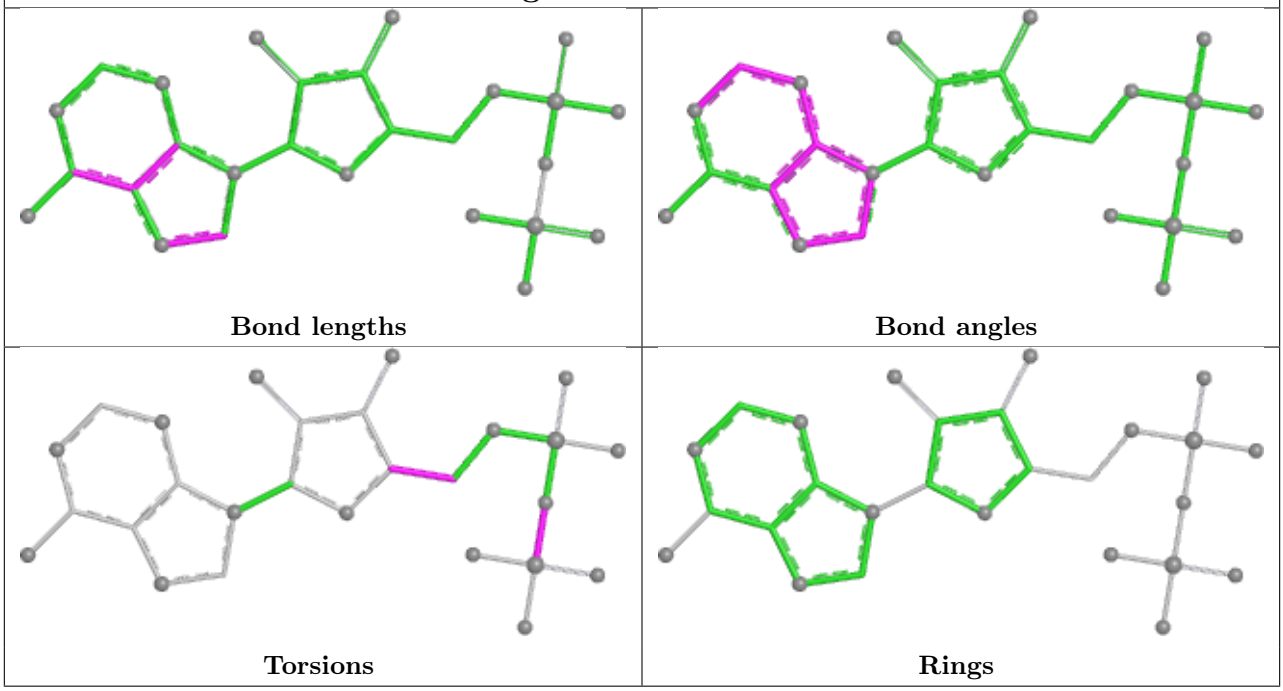
Ligand ADP D 4502



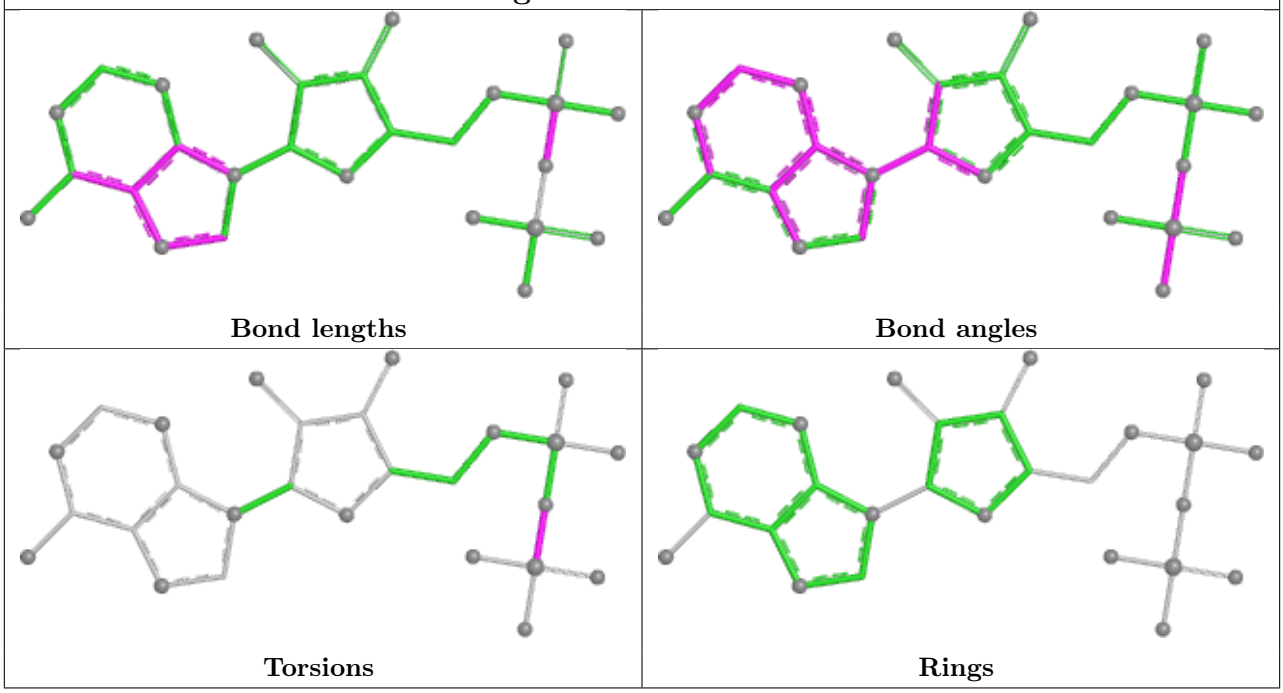
Ligand ADP A 2502



Ligand ADP A 502



Ligand ADP D 3502



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	B	12/15 (80%)	0.30	1 (8%)	17	10	37, 42, 48, 48	0
1	E	12/15 (80%)	0.20	0	100	100	38, 47, 53, 62	0
2	C	6/6 (100%)	0.51	0	100	100	41, 48, 63, 66	1 (16%)
2	F	6/6 (100%)	-0.05	0	100	100	42, 50, 55, 56	1 (16%)
3	A	1609/1706 (94%)	0.37	48 (2%)	52	32	39, 49, 64, 96	0
3	D	1609/1706 (94%)	0.21	25 (1%)	70	50	39, 49, 65, 96	0
All	All	3254/3454 (94%)	0.29	74 (2%)	61	40	37, 49, 64, 96	2 (0%)

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	4291	TYR	3.8
3	A	330	ASN	3.6
3	A	1289	ALA	3.5
3	A	168	ALA	3.5
3	D	4316	ALA	3.4
3	D	4150	THR	3.4
3	D	4068	GLU	3.3
3	A	4194	GLN	3.2
3	A	91	ALA	3.2
3	D	3329	SER	3.2
3	A	326	LEU	3.1
3	A	53	ALA	3.1
3	D	1289	ALA	3.0
3	A	247	VAL	3.0
3	D	176	ARG	3.0
3	A	37	VAL	2.9
3	D	3145	SER	2.9
3	D	4295	GLY	2.9
3	D	4277	LEU	2.9

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Mol	Chain	Res	Type	RSRZ
3	D	4275	VAL	2.8
3	A	328	LEU	2.8
3	A	42	THR	2.8
3	A	299	GLY	2.8
3	A	1298	ILE	2.8
3	A	249	ASN	2.8
3	A	90	CYS	2.7
3	D	4314	GLU	2.7
3	A	113	ASN	2.7
3	A	276	ASP	2.7
3	A	331	PRO	2.6
3	A	212	GLY	2.6
3	D	3095	ALA	2.6
3	A	1287	ALA	2.6
3	A	49	ILE	2.5
3	D	3330	ASN	2.5
3	D	4278	GLY	2.5
3	D	1287	ALA	2.4
3	A	1054	GLY	2.4
3	A	51	LEU	2.4
3	A	3204	GLY	2.4
3	D	4279	VAL	2.4
3	A	324	ARG	2.3
3	A	1291	TYR	2.3
3	A	114	LEU	2.3
3	A	251	ILE	2.3
3	A	128	ILE	2.3
3	A	63	GLU	2.3
3	A	2287	ALA	2.3
3	A	189	LEU	2.2
3	A	60	ARG	2.2
3	D	1235	GLU	2.2
1	B	1002	DT	2.2
3	A	1299	GLY	2.2
3	A	4097	HIS	2.2
3	A	45	LEU	2.2
3	D	4164	MET	2.2
3	A	197	MET	2.2
3	A	4068	GLU	2.2
3	A	4285	GLU	2.2
3	D	3298	ILE	2.1
3	D	1001	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
3	A	52	GLY	2.1
3	A	1002	ILE	2.1
3	A	252	ALA	2.1
3	D	4290	TRP	2.1
3	A	4155	ILE	2.1
3	A	3145	SER	2.1
3	A	55	GLY	2.1
3	A	129	CYS	2.0
3	D	3287	ALA	2.0
3	A	215	LEU	2.0
3	A	4002	ILE	2.0
3	D	2064	ILE	2.0
3	D	4313	PRO	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	0.71	0.14	41,41,43,43	0
5	ALF	A	4501	5/5	0.78	0.13	49,49,51,51	0
4	MG	D	3500	1/1	0.83	0.20	31,31,31,31	0
4	MG	D	500	1/1	0.83	0.17	34,34,34,34	0
4	MG	D	2500	1/1	0.83	0.23	32,32,32,32	0
4	MG	A	500	1/1	0.84	0.17	44,44,44,44	0
5	ALF	A	501	5/5	0.84	0.12	38,39,44,46	0
6	ADP	D	4502	27/27	0.88	0.10	41,43,45,46	0
4	MG	A	1500	1/1	0.89	0.20	38,38,38,38	0
5	ALF	D	3501	5/5	0.90	0.10	27,29,33,33	0

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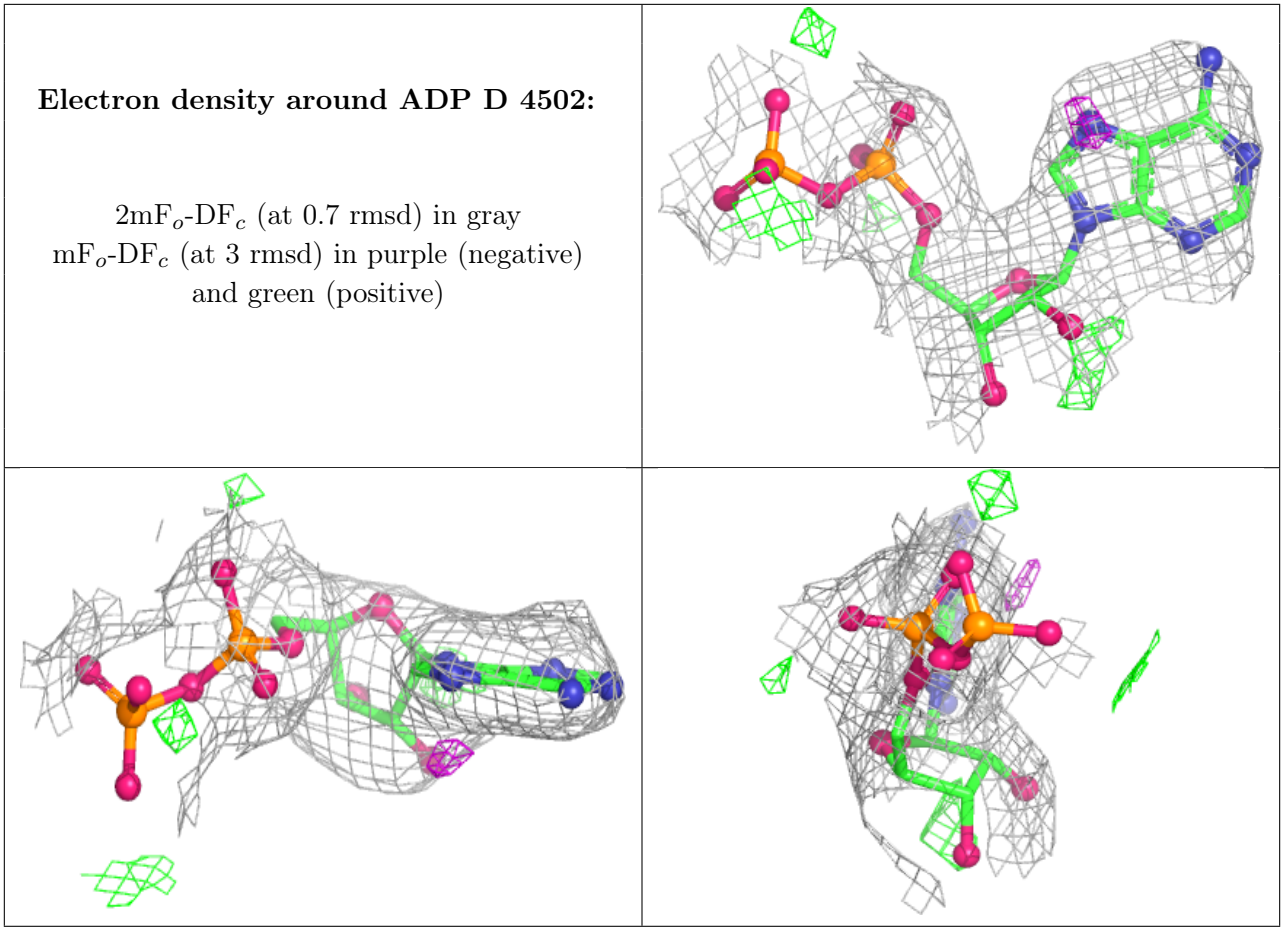
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	ALF	A	1501	5/5	0.90	0.12	35,35,38,41	0
6	ADP	A	502	27/27	0.90	0.09	42,44,48,49	0
6	ADP	A	4502	27/27	0.90	0.09	31,42,44,45	0
4	MG	A	2500	1/1	0.90	0.22	25,25,25,25	0
5	ALF	D	2501	5/5	0.92	0.15	24,26,29,30	0
5	ALF	A	3501	5/5	0.93	0.10	28,28,31,32	0
4	MG	A	3500	1/1	0.93	0.21	27,27,27,27	0
6	ADP	A	1502	27/27	0.94	0.07	27,30,35,35	0
4	MG	D	1500	1/1	0.94	0.19	28,28,28,28	0
6	ADP	D	3502	27/27	0.94	0.09	28,34,36,37	0
5	ALF	A	2501	5/5	0.94	0.10	24,25,27,28	0
5	ALF	D	501	5/5	0.95	0.09	30,30,32,35	0
6	ADP	A	3502	27/27	0.96	0.08	16,20,24,26	0
5	ALF	D	1501	5/5	0.96	0.10	23,24,26,26	0
6	ADP	D	502	27/27	0.96	0.06	16,23,29,30	0
6	ADP	D	2502	27/27	0.96	0.06	25,27,29,30	0
4	MG	A	4500	1/1	0.96	0.13	32,32,32,32	0
4	MG	D	4500	1/1	0.96	0.14	39,39,39,39	0
6	ADP	D	1502	27/27	0.97	0.06	15,19,23,24	0
6	ADP	A	2502	27/27	0.97	0.06	15,20,27,27	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.

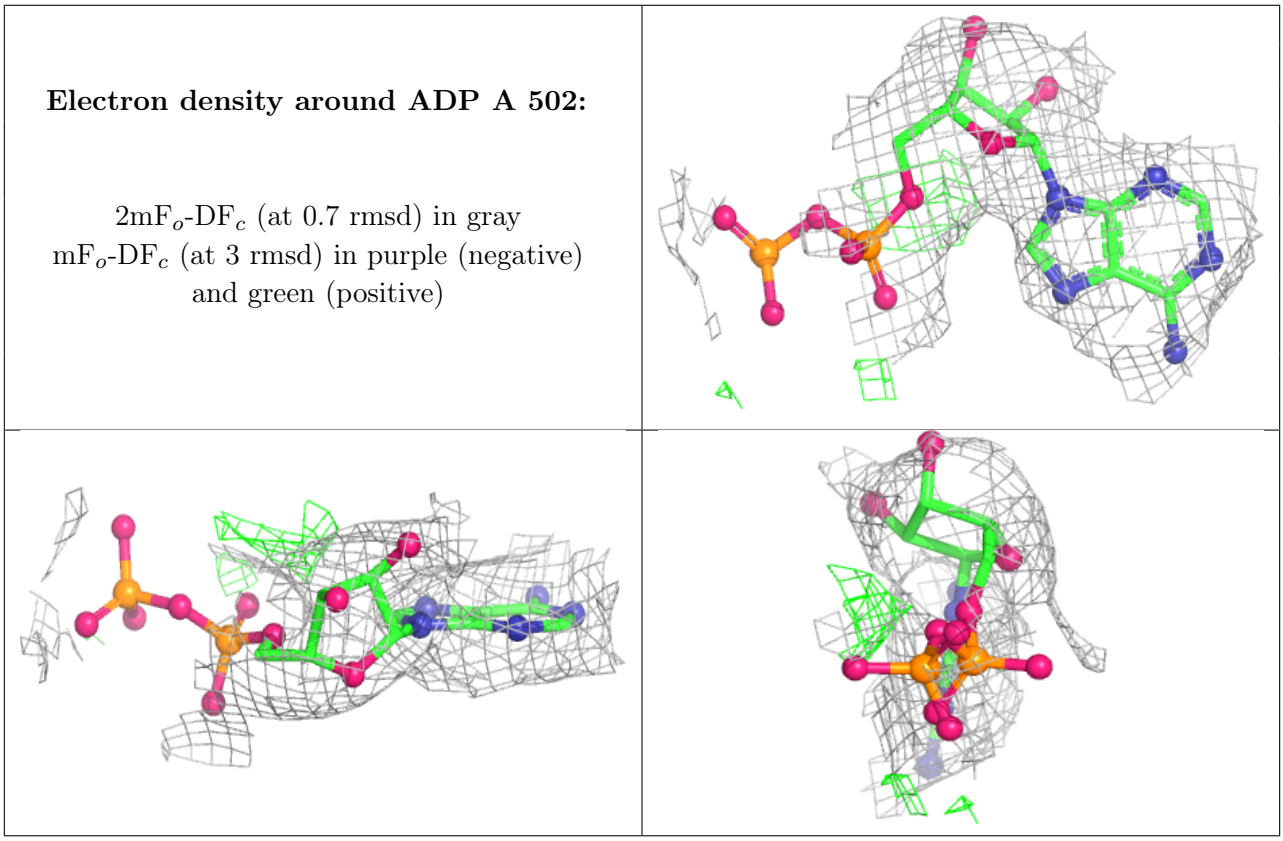
Electron density around ADP D 4502:

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



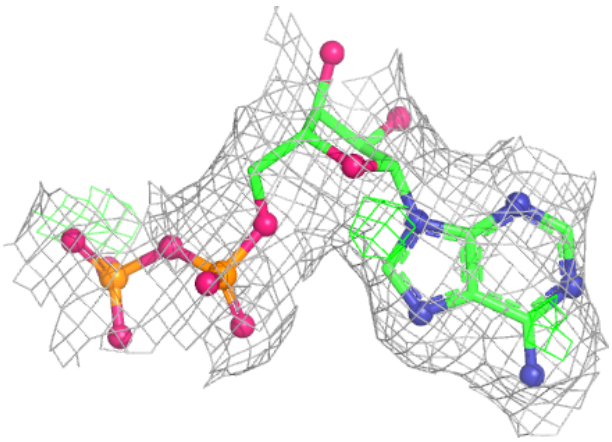
Electron density around ADP A 502:

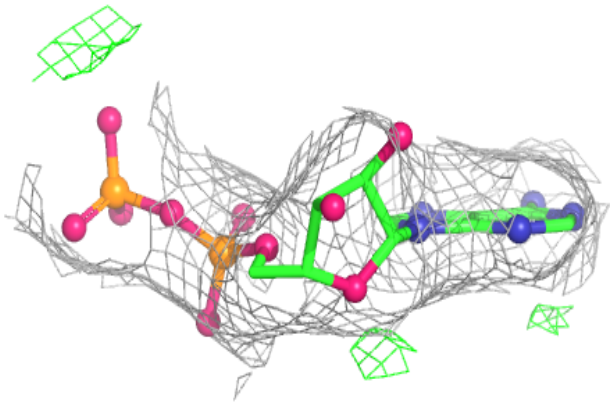
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

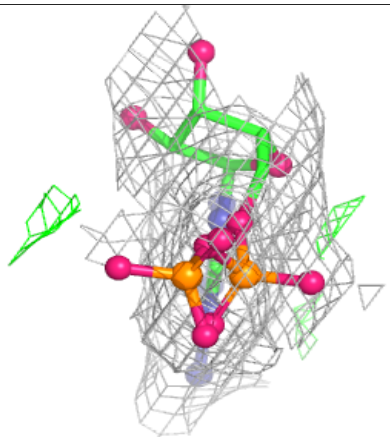


Electron density around ADP A 4502:

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

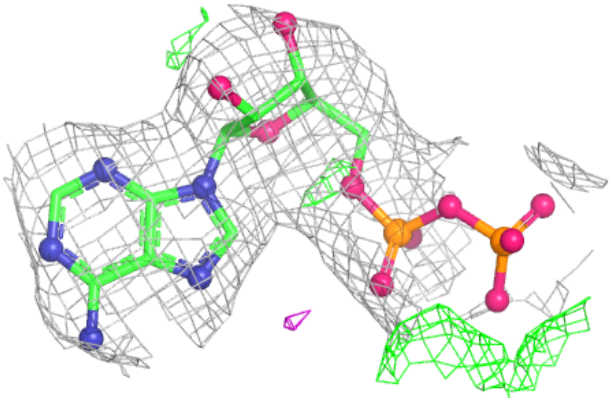


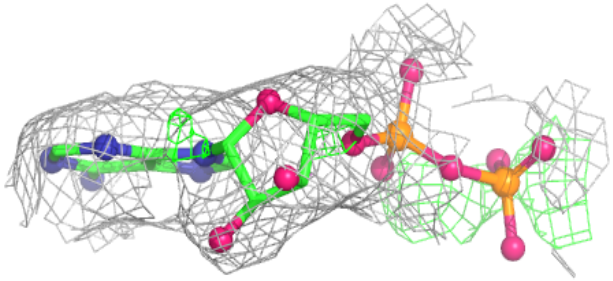


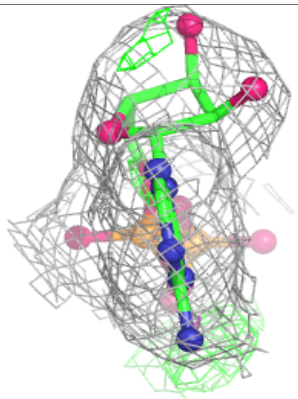


Electron density around ADP A 1502:

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

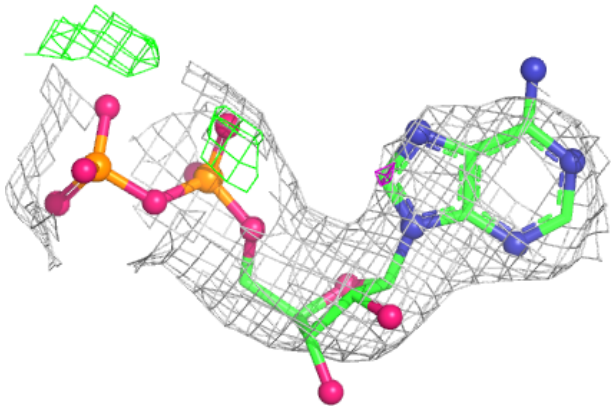


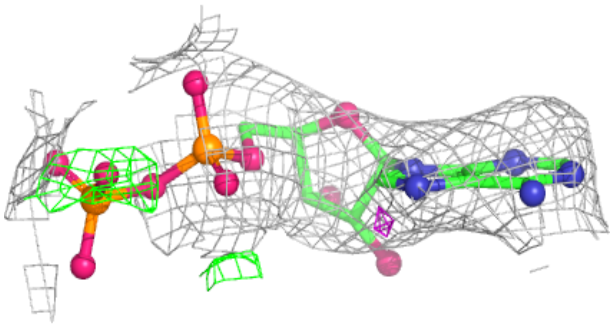


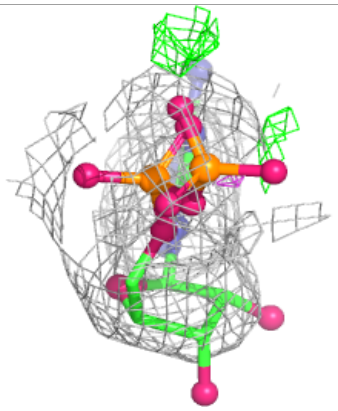


Electron density around ADP D 3502:

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

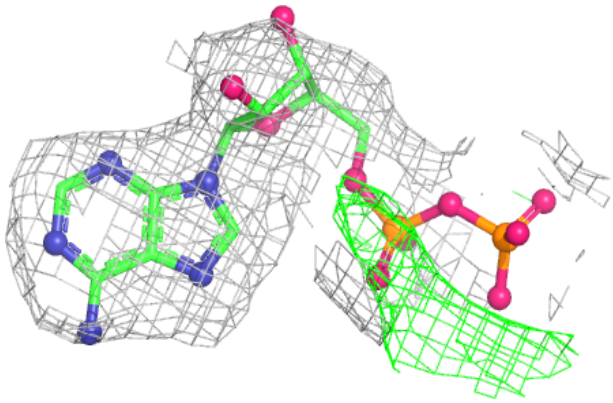


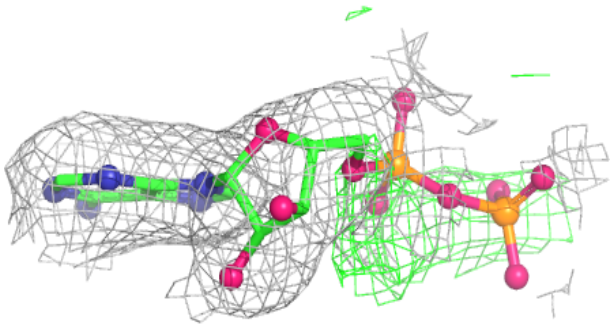


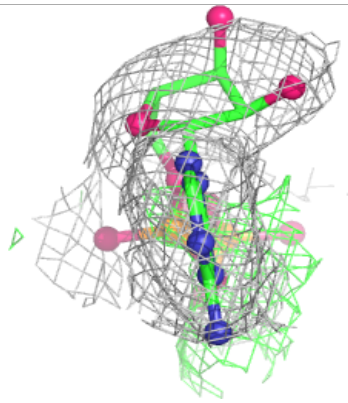


Electron density around ADP A 3502:

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

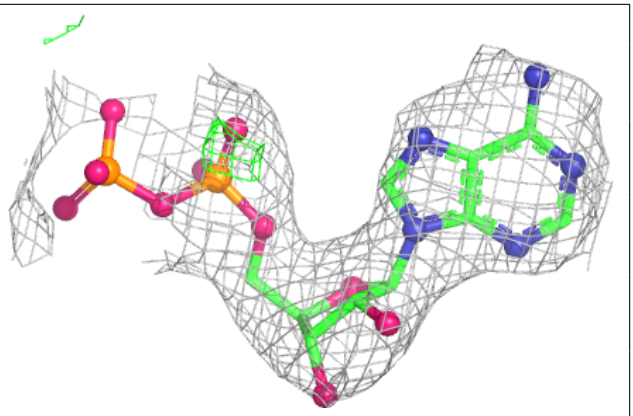


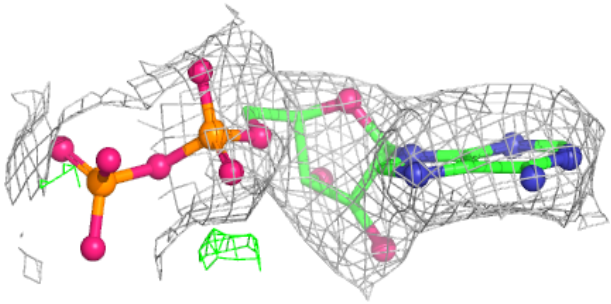


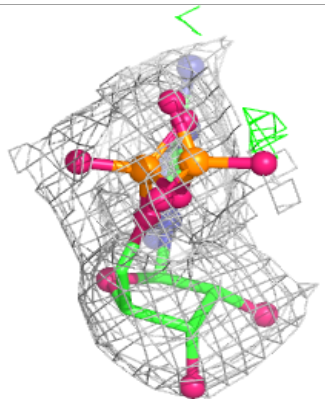


Electron density around ADP D 502:

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

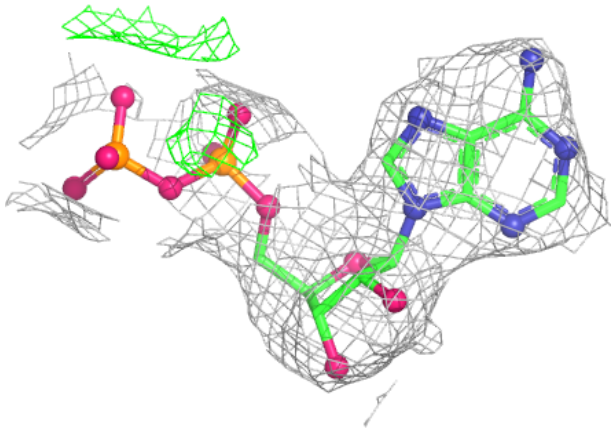


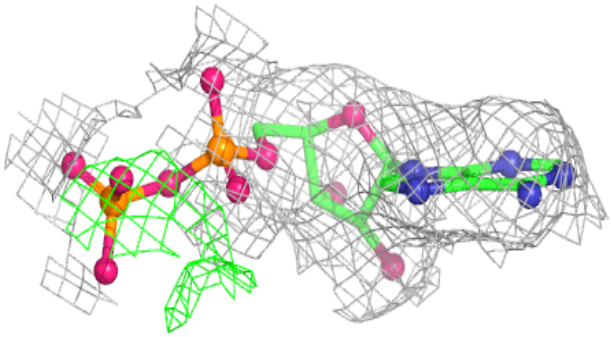


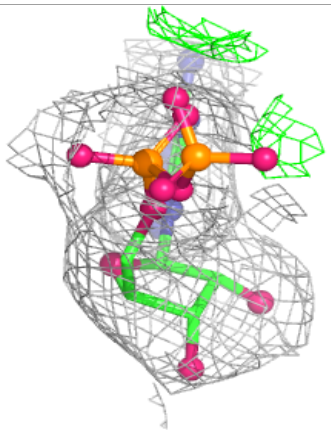


Electron density around ADP D 2502:

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

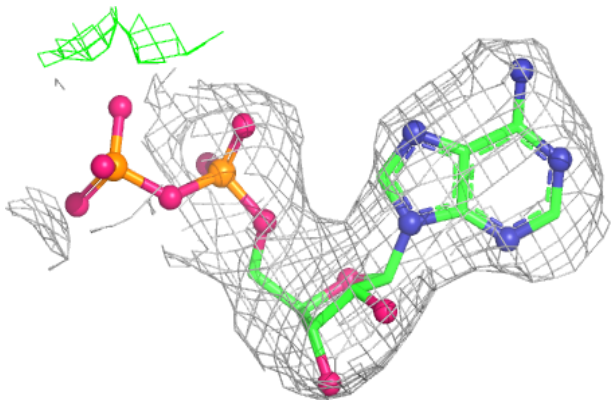


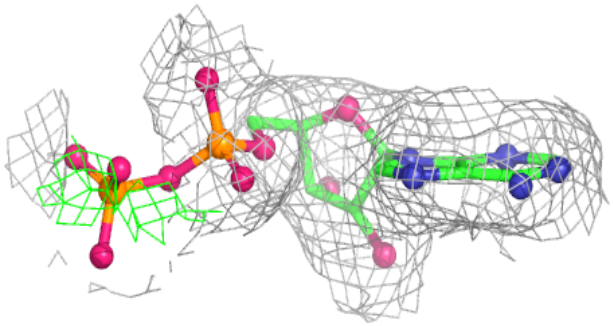


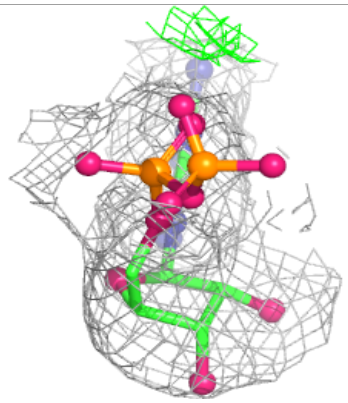


Electron density around ADP D 1502:

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

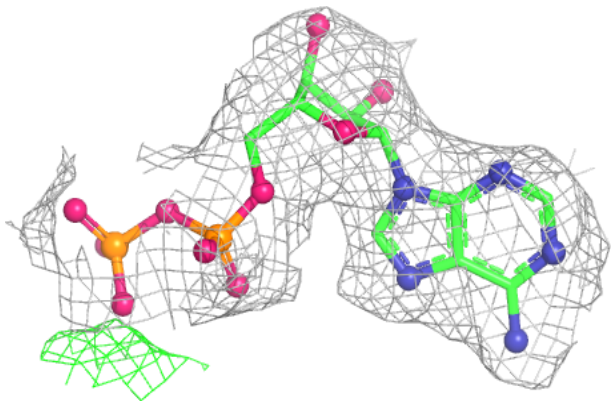


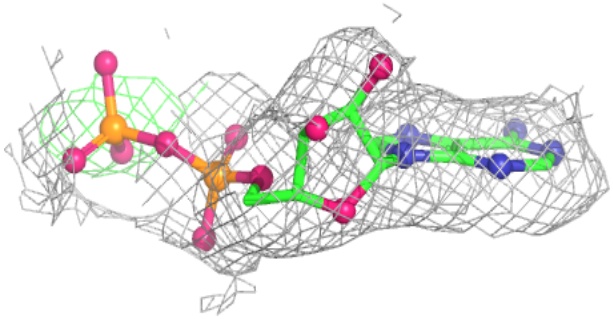


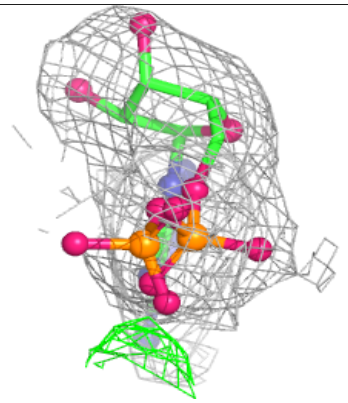


Electron density around ADP A 2502:

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







6.5 Other polymers (i)

There are no such residues in this entry.