Full wwPDB X-ray Structure Validation Report (i)

Feb 11, 2024 – 10:07 AM EST

PDB ID	:	3CMX
Title	:	Mechanism of homologous recombination from the RecA-ssDNA/dsDNA structures
Authors	:	Pavletich, N.P.
Deposited on	:	2008-03-24
Resolution	:	3.40 Å(reported)

This is a 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:

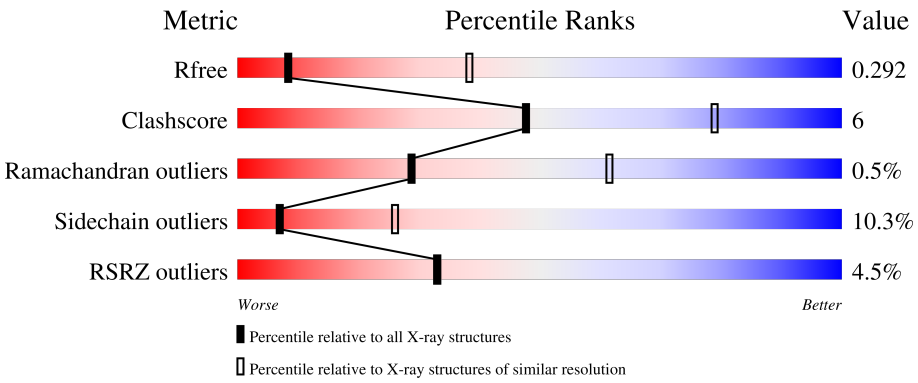
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1026 (3.48-3.32)
Clashscore	141614	1055 (3.48-3.32)
Ramachandran outliers	138981	1038 (3.48-3.32)
Sidechain outliers	138945	1038 (3.48-3.32)
RSRZ outliers	127900	2173 (3.50-3.30)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments 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	20% 40% 27% 13%
1	E	15	20% 33% 33% 13%
2	C	12	42% 75% 17% 8%
2	F	12	92% 92% 8%
3	A	1706	4% 78% 14% • 6%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
3	D	1706	3% 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*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
1	B	13	260	130	26	91	13	0	0	0
1	E	13	260	130	26	91	13	0	0	0

- 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
			Total	C	N	O	P			
2	C	11	211	100	50	51	10	0	0	0
2	F	12	232	110	55	56	11	0	0	0

- Molecule 3 is a protein called Protein recA.

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

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

Continued on next page...

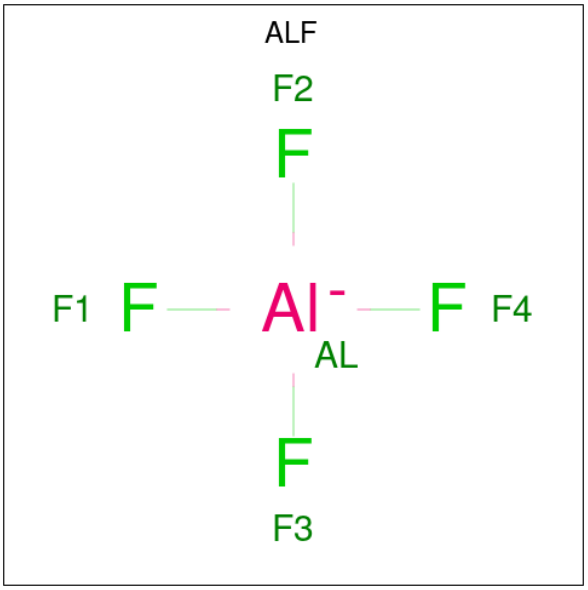
Continued from previous page...

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

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

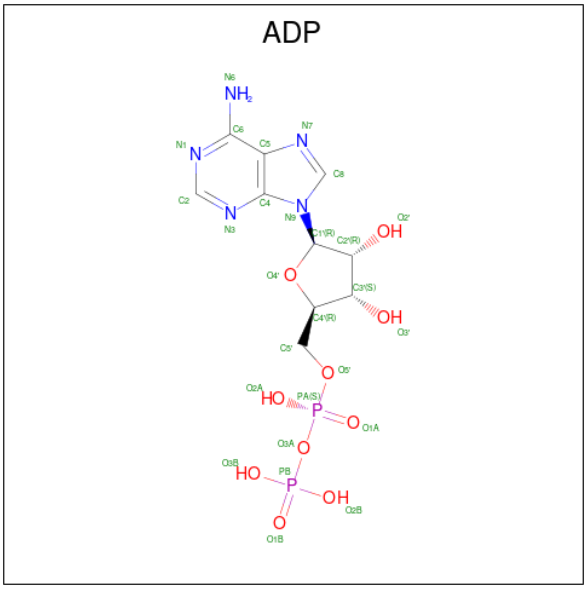
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	5	5	5	0	0
			Total	Mg		
4	D	5	5	5	0	0

- Molecule 5 is TETRAFLUOROALUMINATE ION (three-letter code: 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 (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



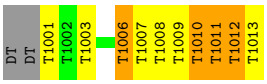
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
6	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
6	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
6	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
6	A	1	27	10	5	10	2	0	0
			Total	C	N	O	P		
6	D	1	27	10	5	10	2	0	0
			Total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

Chain B: 20% 40% 27% 13%

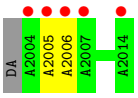


• Molecule 1: DNA (5'-D(*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DTP*DT)-3')

Chain E: 20% 33% 33% 13%

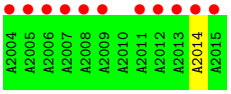
• Molecule 2: DNA (5'-D(*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DA)-3')

Chain C: 42% 75% 17% 8%



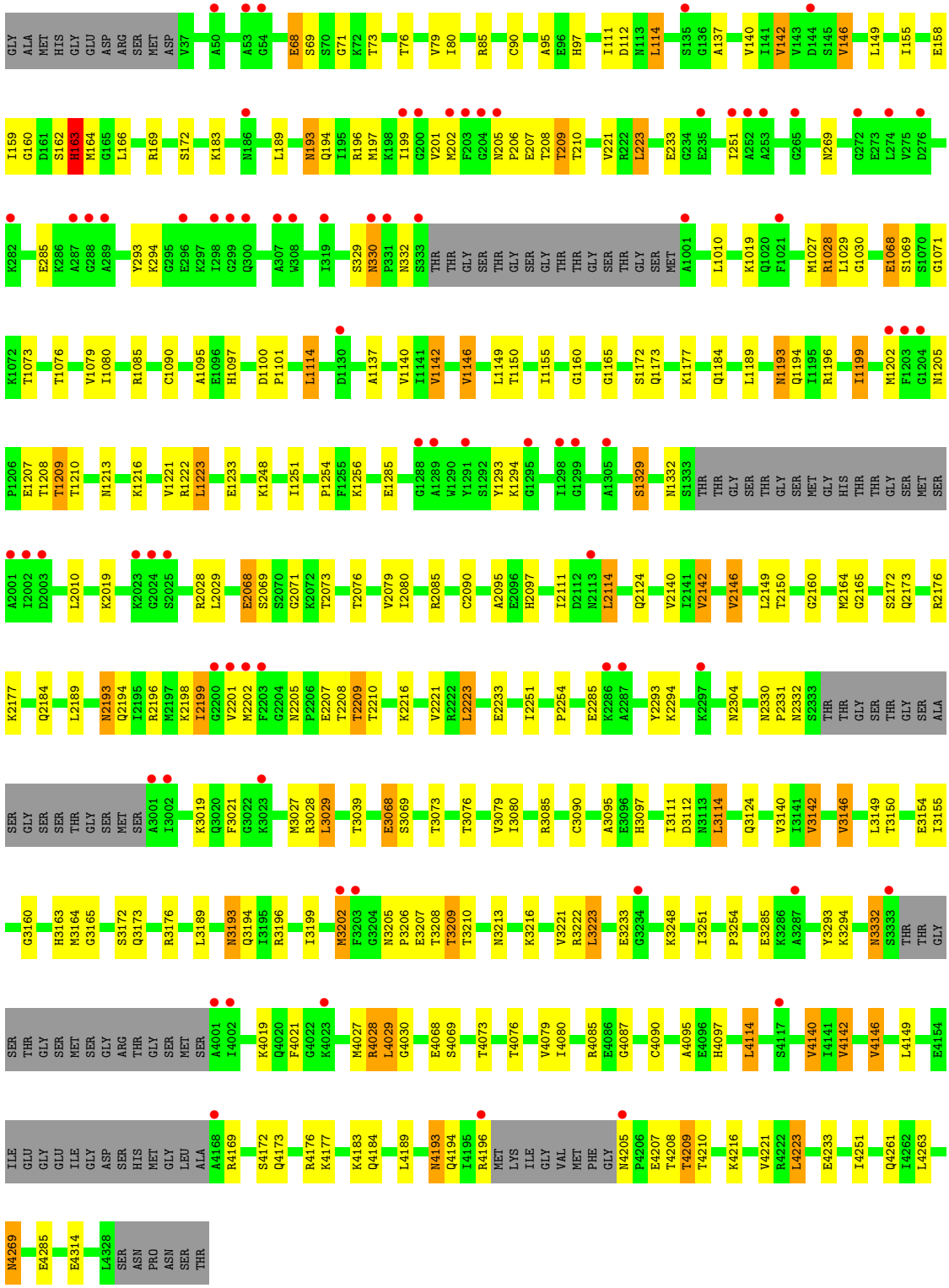
• Molecule 2: DNA (5'-D(*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DAP*DA)-3')

Chain F: 92% 92% 8%



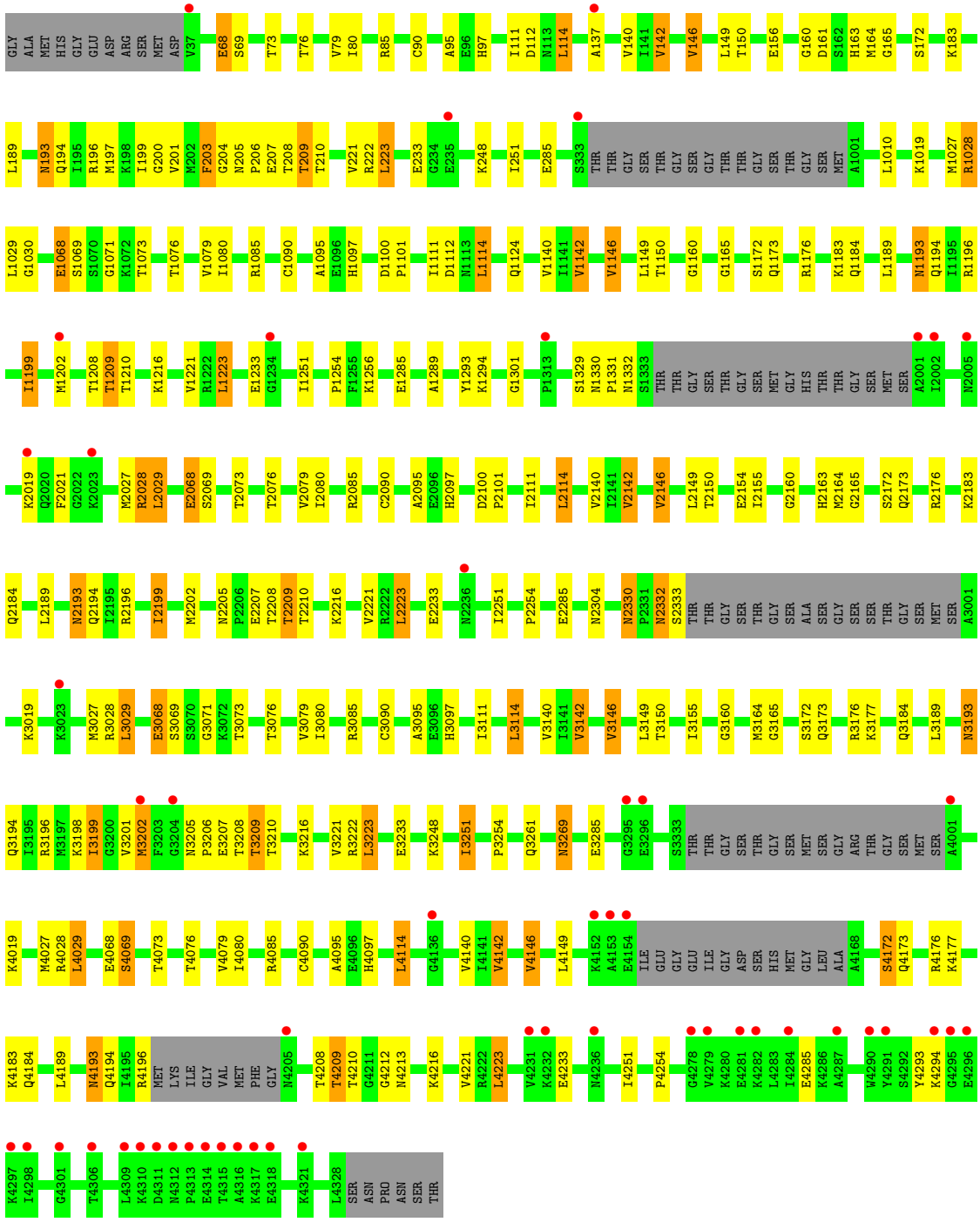
• Molecule 3: Protein recA

Chain A: 4% 78% 14% • 6%



- Molecule 3: Protein recA

Chain D:


GLY ALA MET HIS GLY GLU ASP ARG SER MET ASP V37 E68 S69 T73 T76 V79 I80 R85 C90 A95 E96 H97 I111 D112 N113 L114 A137 V140 I141 V142 V146 L149 T150 E156 G160 D161 S162 H163 M164 G165 S172 K183
L189 N193 Q194 I195 R196 M197 K198 I199 G200 V201 M202 F203 G204 N205 P206 E207 T208 T209 T210 V221 R222 L223 E233 G234 E235 K248 I251 E285 S333 THR THR GLY SER THR GLY SER GLY THR THR GLY SER THR GLY SER MET A1001 L1010 K1019 M1027 R1028
L1029 G1030 E1068 S1069 S1070 G1071 K1072 T1073 T1076 V1079 I1080 R1085 C1090 A1095 E1096 H1097 D1100 P1101 I1111 D1112 N1113 L1114 Q1124 V1140 I1141 V1142 V1146 L1149 T1150 G1160 G1165 S1172 Q1173 R1176 K1183 Q1184 L1189 N1193 Q1194 I1195 R1196
I1199 M1202 T1208 T1209 T1210 K1216 V1221 R1222 L1223 E1233 G1234 I1251 P1254 F1255 K1256 E1285 A1289 Y1293 K1294 G1301 P1313 S1329 N1330 P1331 N1332 S1333 THR THR GLY SER THR GLY SER MET GLY HIS THR THR GLY SER MET SER A2001 T2002 N2005
K2019 Q2020 F2021 G2022 K2023 M2027 R2028 L2029 E2068 S2069 T2073 T2076 V2079 I2080 R2085 C2090 A2095 E2096 H2097 D2100 P2101 I2111 L2114 V2140 I2141 V2142 V2146 L2149 T2150 E2154 I2155 G2160 H2163 M2164 G2165 S2172 Q2173 R2176 K2183
Q2184 L2189 N2193 Q2194 I2195 R2196 I2199 M2202 N2205 P2206 E2207 T2208 T2209 T2210 K2216 V2221 R2222 L2223 E2233 N2236 I2251 P2254 E2285 N2304 N2330 P2331 N2332 S2333 THR THR GLY SER THR GLY SER ALA SER GLY SER SER THR GLY SER MET SER A3001
K3019 K3023 M3027 R3028 L3029 E3068 S3069 S3070 G3071 K3072 T3073 T3076 V3079 I3080 R3085 C3090 A3095 E3096 H3097 I3111 L3114 V3140 I3141 V3142 V3146 L3149 T3150 I3155 G3160 M3164 G3165 S3172 Q3173 R3176 K3177 Q3184 L3189 N3193
Q3194 I3195 R3196 M3197 K3198 I3199 G3200 V3201 M3202 F3203 G3204 N3205 P3206 E3207 T3208 T3209 T3210 K3216 V3221 R3222 L3223 E3233 K3248 I3251 P3254 Q3261 N3269 E3285 G3295 E3296 S3333 THR THR GLY SER THR GLY SER MET SER GLY ARG THR GLY SER MET SER A4001
K4019 M4027 R4028 L4029 E4068 S4069 T4073 T4076 V4079 I4080 R4085 C4090 A4095 E4096 H4097 L4114 G4136 V4140 I4141 V4142 V4146 L4149 K4152 A4153 E4154 ILE GLU GLY GLU ILE GLY ASP SER HIS MET GLY LEU ALA A4168 S4172 Q4173 R4176 K4177
K4183 Q4184 L4189 N4193 Q4194 I4195 R4196 MET LYS ILE GLY VAL MET PHE GLY N4205 T4208 T4209 T4210 G4211 G4212 N4213 K4216 V4221 R4222 L4223 V4231 K4232 E4233 N4236 I4251 P4254 G4278 V4279 K4280 E4281 K4282 L4283 T4284 E4285 K4286 A4287 W4290 Y4291 S4292 Y4293 K4294 G4295 E4296
K4297 I4298 G4301 T4306 L4309 K4310 D4311 N4312 P4313 E4314 T4315 A4316 K4317 E4318 K4321 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 – 3.40 39.75 – 3.40	Depositor EDS
% Data completeness (in resolution range)	94.7 (40.00-3.40) 94.7 (39.75-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.47 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.3.0036	Depositor
R, R_{free}	0.238 , 0.256 0.279 , 0.292	Depositor DCC
R_{free} test set	1623 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å^2)	83.1	Xtriage
Anisotropy	0.082	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 4.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.41$, $< L^2 > = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.86	EDS
Total number of atoms	25459	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% of the height of the origin peak. No significant pseudotranslation is detected.*

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

All (1) bond length outliers are listed below:

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

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	1012	DT	C4-C5-C7	8.48	124.09	119.00
1	E	1009	DT	C4-C5-C7	8.41	124.05	119.00
1	B	1006	DT	C4-C5-C7	8.17	123.90	119.00
1	B	1009	DT	C4-C5-C7	8.03	123.82	119.00
2	F	2014	DA	C1'-O4'-C4'	-7.97	102.13	110.10
1	E	1012	DT	C4-C5-C7	7.65	123.59	119.00
1	E	1003	DT	O4'-C4'-C3'	-7.39	101.54	104.50
1	E	1006	DT	C4-C5-C7	7.29	123.38	119.00
1	B	1009	DT	C6-C5-C7	-7.01	118.69	122.90
1	B	1012	DT	C6-C5-C7	-6.85	118.79	122.90
1	E	1012	DT	C6-C5-C7	-6.64	118.92	122.90
1	E	1009	DT	C6-C5-C7	-6.58	118.95	122.90
2	F	2014	DA	O4'-C1'-N9	6.17	112.32	108.00
1	B	1006	DT	C6-C5-C7	-6.00	119.30	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	1006	DT	C6-C5-C7	-5.97	119.32	122.90
1	E	1003	DT	C4-C5-C7	5.94	122.56	119.00
1	B	1003	DT	C4-C5-C7	5.72	122.43	119.00
1	B	1011	DT	C4-C5-C7	5.62	122.37	119.00
1	E	1011	DT	C4-C5-C7	5.39	122.23	119.00
2	F	2014	DA	N1-C6-N6	5.34	121.81	118.60
1	E	1008	DT	C4-C5-C7	5.23	122.14	119.00
1	B	1001	DT	P-O3'-C3'	5.20	125.94	119.70
1	E	1013	DT	C6-C5-C7	-5.17	119.80	122.90
1	B	1010	DT	C5-C4-O4	-5.16	121.29	124.90
2	C	2005	DA	O4'-C1'-N9	5.08	111.56	108.00
1	E	1003	DT	C6-C5-C7	-5.06	119.86	122.90
1	E	1004	DT	C5-C4-O4	-5.01	121.39	124.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	260	0	157	7	0
1	E	260	0	157	13	0
2	C	211	0	111	1	0
2	F	232	0	122	0	0
3	A	12083	0	12406	158	1
3	D	12083	0	12406	162	0
4	A	5	0	0	0	0
4	D	5	0	0	0	0
5	A	25	0	0	1	0
5	D	25	0	0	0	0
6	A	135	0	60	7	0
6	D	135	0	60	7	0
All	All	25459	0	25479	313	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (313) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:76:THR:HG21	3:D:142:VAL:HG21	1.46	0.95
3:A:4076:THR:HG21	3:A:4142:VAL:HG21	1.48	0.95
3:D:68:GLU:HG2	3:D:1216:LYS:HB3	1.47	0.95
3:D:2076:THR:HG21	3:D:2142:VAL:HG21	1.49	0.94
3:A:2076:THR:HG21	3:A:2142:VAL:HG21	1.51	0.93
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: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
3:A:2304:ASN:HD21	3:D:2304:ASN:CG	1.82	0.84
1:E:1013:DT:C7	3:D:3199:ILE:HB	2.07	0.83
3:A:4193:ASN:HD22	3:A:4194:GLN:H	1.25	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:2304:ASN:CG	3:D:2304:ASN:HD21	1.87	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:D:76:THR:CG2	3:D:142:VAL:HG21	2.23	0.68
3:D:203:PHE:CG	3:D:204:GLY:N	2.61	0.68
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:A:1068:GLU:HG2	3:A:2216:LYS:HB3	1.77	0.66
3:A:1076:THR:CG2	3:A:1142:VAL:HG21	2.25	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:2076:THR:CG2	3:D:2142:VAL:HG21	2.26	0.65
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:3039:THR:OG1	3:A:3332:ASN:ND2	2.38	0.56
3:D:150:THR:OG1	3:D:1176:ARG:HB3	2.07	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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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: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:162:SER:C	3:A:163:HIS:CG	2.87	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: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
3:D:3193:ASN:OD1	3:D:3209:THR:HG23	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1146:VAL:HA	3:D:1149:LEU:HD22	1.97	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:A:205:ASN:ND2	3:A:207:GLU:HB2	2.31	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:D:4193:ASN:OD1	3:D:4209:THR:HG23	2.16	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
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:D:3146:VAL:HA	3:D:3149:LEU:HD22	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:2332:ASN:CG	3:D:2333:SER:H	2.19	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:A:163:HIS:O	3:A:164:MET:C	2.56	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1111:ILE:HG23	3:D:2029:LEU:HD13	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: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: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: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
3:A:1213:ASN:OD1	3:A:1216:LYS:HE2	2.20	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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%)	29	61
3	D	1589/1706 (93%)	1501 (94%)	81 (5%)	7 (0%)	34	67
All	All	3178/3412 (93%)	2995 (94%)	168 (5%)	15 (0%)	29	61

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
3	D	3165	GLY
3	A	1165	GLY
3	A	163	HIS
3	A	330	ASN

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

All (260) 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	79	VAL
3	A	85	ARG
3	A	114	LEU
3	A	140	VAL
3	A	142	VAL
3	A	146	VAL
3	A	158	GLU
3	A	163	HIS
3	A	172	SER
3	A	183	LYS
3	A	189	LEU
3	A	193	ASN
3	A	197	MET
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	233	GLU
3	A	251	ILE
3	A	285	GLU
3	A	332	ASN
3	A	1019	LYS
3	A	1027	MET
3	A	1028	ARG
3	A	1029	LEU
3	A	1068	GLU
3	A	1069	SER
3	A	1073	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	1172	SER
3	A	1184	GLN
3	A	1189	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	1193	ASN
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	1233	GLU
3	A	1251	ILE
3	A	1285	GLU
3	A	1329	SER
3	A	2019	LYS
3	A	2028	ARG
3	A	2029	LEU
3	A	2068	GLU
3	A	2069	SER
3	A	2073	THR
3	A	2079	VAL
3	A	2085	ARG
3	A	2114	LEU
3	A	2140	VAL
3	A	2142	VAL
3	A	2146	VAL
3	A	2172	SER
3	A	2184	GLN
3	A	2189	LEU
3	A	2193	ASN
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	2233	GLU
3	A	2251	ILE
3	A	2285	GLU
3	A	2332	ASN
3	A	3019	LYS
3	A	3027	MET
3	A	3028	ARG
3	A	3029	LEU
3	A	3068	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	3069	SER
3	A	3073	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	3172	SER
3	A	3189	LEU
3	A	3193	ASN
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	3233	GLU
3	A	3251	ILE
3	A	3285	GLU
3	A	3332	ASN
3	A	4019	LYS
3	A	4027	MET
3	A	4028	ARG
3	A	4029	LEU
3	A	4068	GLU
3	A	4069	SER
3	A	4073	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	4172	SER
3	A	4183	LYS
3	A	4184	GLN
3	A	4189	LEU
3	A	4193	ASN
3	A	4208	THR
3	A	4209	THR
3	A	4210	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	A	4223	LEU
3	A	4233	GLU
3	A	4251	ILE
3	A	4285	GLU
3	D	68	GLU
3	D	69	SER
3	D	73	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	156	GLU
3	D	161	ASP
3	D	172	SER
3	D	183	LYS
3	D	189	LEU
3	D	193	ASN
3	D	197	MET
3	D	203	PHE
3	D	208	THR
3	D	209	THR
3	D	210	THR
3	D	223	LEU
3	D	233	GLU
3	D	251	ILE
3	D	285	GLU
3	D	1019	LYS
3	D	1027	MET
3	D	1028	ARG
3	D	1029	LEU
3	D	1068	GLU
3	D	1069	SER
3	D	1073	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	1172	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	1183	LYS
3	D	1184	GLN
3	D	1189	LEU
3	D	1193	ASN
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	1233	GLU
3	D	1251	ILE
3	D	1285	GLU
3	D	2019	LYS
3	D	2027	MET
3	D	2028	ARG
3	D	2029	LEU
3	D	2068	GLU
3	D	2069	SER
3	D	2073	THR
3	D	2079	VAL
3	D	2085	ARG
3	D	2114	LEU
3	D	2140	VAL
3	D	2142	VAL
3	D	2146	VAL
3	D	2172	SER
3	D	2183	LYS
3	D	2184	GLN
3	D	2189	LEU
3	D	2193	ASN
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	2233	GLU
3	D	2251	ILE
3	D	2285	GLU
3	D	2330	ASN
3	D	3019	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	3027	MET
3	D	3028	ARG
3	D	3029	LEU
3	D	3068	GLU
3	D	3069	SER
3	D	3073	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	3172	SER
3	D	3184	GLN
3	D	3189	LEU
3	D	3193	ASN
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	3233	GLU
3	D	3251	ILE
3	D	3285	GLU
3	D	4019	LYS
3	D	4027	MET
3	D	4028	ARG
3	D	4029	LEU
3	D	4068	GLU
3	D	4069	SER
3	D	4073	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	4172	SER
3	D	4183	LYS
3	D	4184	GLN
3	D	4189	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	D	4193	ASN
3	D	4208	THR
3	D	4209	THR
3	D	4210	THR
3	D	4223	LEU
3	D	4233	GLU
3	D	4251	ILE
3	D	4285	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (83) such sidechains are listed below:

Mol	Chain	Res	Type
3	A	97	HIS
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	1124	GLN
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	2097	HIS
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	2330	ASN
3	A	3097	HIS
3	A	3124	GLN
3	A	3173	GLN
3	A	3181	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	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	1300	GLN
3	D	1304	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	4300	GLN
3	D	4304	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides 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	1501	-	0,4,4	-	-	-		
6	ADP	D	3502	4	24,29,29	1.14	2 (8%)	29,45,45	1.41	5 (17%)
5	ALF	A	501	-	0,4,4	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	ALF	D	501	-	0,4,4	-	-	-		
6	ADP	D	502	4	24,29,29	1.09	2 (8%)	29,45,45	1.31	5 (17%)
5	ALF	D	1501	-	0,4,4	-	-	-		
5	ALF	D	2501	-	0,4,4	-	-	-		
5	ALF	A	2501	-	0,4,4	-	-	-		
6	ADP	A	2502	4	24,29,29	1.02	1 (4%)	29,45,45	1.39	5 (17%)
6	ADP	A	1502	4	24,29,29	0.96	1 (4%)	29,45,45	1.42	5 (17%)
6	ADP	A	502	4	24,29,29	1.16	3 (12%)	29,45,45	1.49	3 (10%)
5	ALF	D	3501	-	0,4,4	-	-	-		
5	ALF	D	4501	-	0,4,4	-	-	-		
6	ADP	D	4502	4	24,29,29	1.15	3 (12%)	29,45,45	1.28	3 (10%)
6	ADP	A	4502	-	24,29,29	0.99	1 (4%)	29,45,45	1.37	4 (13%)
6	ADP	A	3502	4	24,29,29	1.01	1 (4%)	29,45,45	1.33	4 (13%)
6	ADP	D	2502	4	24,29,29	1.14	2 (8%)	29,45,45	1.39	5 (17%)
5	ALF	A	3501	-	0,4,4	-	-	-		
5	ALF	A	4501	-	0,4,4	-	-	-		
6	ADP	D	1502	4	24,29,29	1.04	2 (8%)	29,45,45	1.28	4 (13%)

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

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	3502	ADP	C5-C4	3.04	1.49	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2502	ADP	C5-C4	3.03	1.48	1.40
6	D	4502	ADP	C5-C4	2.92	1.48	1.40
6	D	502	ADP	C5-C4	2.91	1.48	1.40
6	A	502	ADP	C5-C4	2.79	1.48	1.40
6	D	1502	ADP	C5-C4	2.68	1.48	1.40
6	A	4502	ADP	C5-C4	2.65	1.48	1.40
6	A	502	ADP	C2-N3	2.50	1.36	1.32
6	A	3502	ADP	C5-C4	2.43	1.47	1.40
6	D	2502	ADP	O4'-C1'	2.42	1.44	1.41
6	A	2502	ADP	C5-C4	2.42	1.47	1.40
6	A	1502	ADP	C5-C4	2.36	1.47	1.40
6	D	4502	ADP	C2-N3	2.31	1.35	1.32
6	D	502	ADP	O4'-C1'	2.28	1.44	1.41
6	D	4502	ADP	C2'-C1'	-2.17	1.50	1.53
6	D	3502	ADP	O4'-C1'	2.08	1.44	1.41
6	D	1502	ADP	C2-N3	2.02	1.35	1.32
6	A	502	ADP	C4-N3	2.00	1.38	1.35

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	502	ADP	N3-C2-N1	-4.32	121.93	128.68
6	A	502	ADP	PA-O3A-PB	-3.58	120.53	132.83
6	A	2502	ADP	N3-C2-N1	-3.51	123.19	128.68
6	A	4502	ADP	N3-C2-N1	-3.45	123.29	128.68
6	A	1502	ADP	N3-C2-N1	-3.39	123.38	128.68
6	A	3502	ADP	N3-C2-N1	-3.31	123.51	128.68
6	D	2502	ADP	N3-C2-N1	-3.29	123.53	128.68
6	D	1502	ADP	C4-C5-N7	-3.23	106.04	109.40
6	D	3502	ADP	N3-C2-N1	-3.11	123.81	128.68
6	D	502	ADP	N3-C2-N1	-2.94	124.09	128.68
6	A	2502	ADP	PA-O3A-PB	-2.93	122.77	132.83
6	D	4502	ADP	PA-O3A-PB	-2.82	123.16	132.83
6	A	4502	ADP	PA-O3A-PB	-2.75	123.38	132.83
6	A	1502	ADP	N6-C6-N1	2.69	124.16	118.57
6	D	2502	ADP	C2-N1-C6	2.69	123.36	118.75
6	D	4502	ADP	N3-C2-N1	-2.69	124.48	128.68
6	D	3502	ADP	C2-N1-C6	2.59	123.19	118.75
6	A	1502	ADP	O3'-C3'-C4'	-2.59	103.57	111.05
6	A	4502	ADP	C2-N1-C6	2.58	123.16	118.75
6	A	1502	ADP	O2B-PB-O3A	-2.57	96.03	104.64
6	D	1502	ADP	N3-C2-N1	-2.52	124.75	128.68

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	A	4502	ADP	N6-C6-N1	2.43	123.61	118.57
6	D	1502	ADP	O2B-PB-O3A	-2.37	96.68	104.64
6	D	502	ADP	PA-O3A-PB	-2.37	124.69	132.83
6	A	3502	ADP	O2B-PB-O3A	-2.36	96.71	104.64
6	D	4502	ADP	N6-C6-N1	2.34	123.44	118.57
6	D	3502	ADP	PA-O3A-PB	-2.34	124.80	132.83
6	A	3502	ADP	PA-O3A-PB	-2.27	125.03	132.83
6	D	502	ADP	O2B-PB-O3A	-2.26	97.05	104.64
6	A	2502	ADP	C3'-C2'-C1'	2.24	104.36	100.98
6	D	1502	ADP	PA-O3A-PB	-2.21	125.24	132.83
6	D	2502	ADP	O2B-PB-O3A	-2.17	97.36	104.64
6	D	3502	ADP	O2B-PB-O3A	-2.12	97.54	104.64
6	D	2502	ADP	PA-O3A-PB	-2.11	125.59	132.83
6	D	502	ADP	C2-N1-C6	2.10	122.35	118.75
6	D	502	ADP	O2A-PA-O1A	2.06	122.44	112.24
6	A	2502	ADP	C4-C5-N7	-2.05	107.26	109.40
6	D	3502	ADP	N6-C6-N1	2.05	122.83	118.57
6	A	502	ADP	O2A-PA-O1A	2.04	122.32	112.24
6	A	3502	ADP	O4'-C1'-C2'	-2.03	103.96	106.93
6	D	2502	ADP	O3'-C3'-C4'	-2.03	105.19	111.05
6	A	1502	ADP	C2-N1-C6	2.01	122.19	118.75
6	A	2502	ADP	O2B-PB-O3A	-2.01	97.89	104.64

There are no chirality outliers.

All (26) torsion outliers are listed below:

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
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	A	4502	ADP	C3'-C4'-C5'-O5'

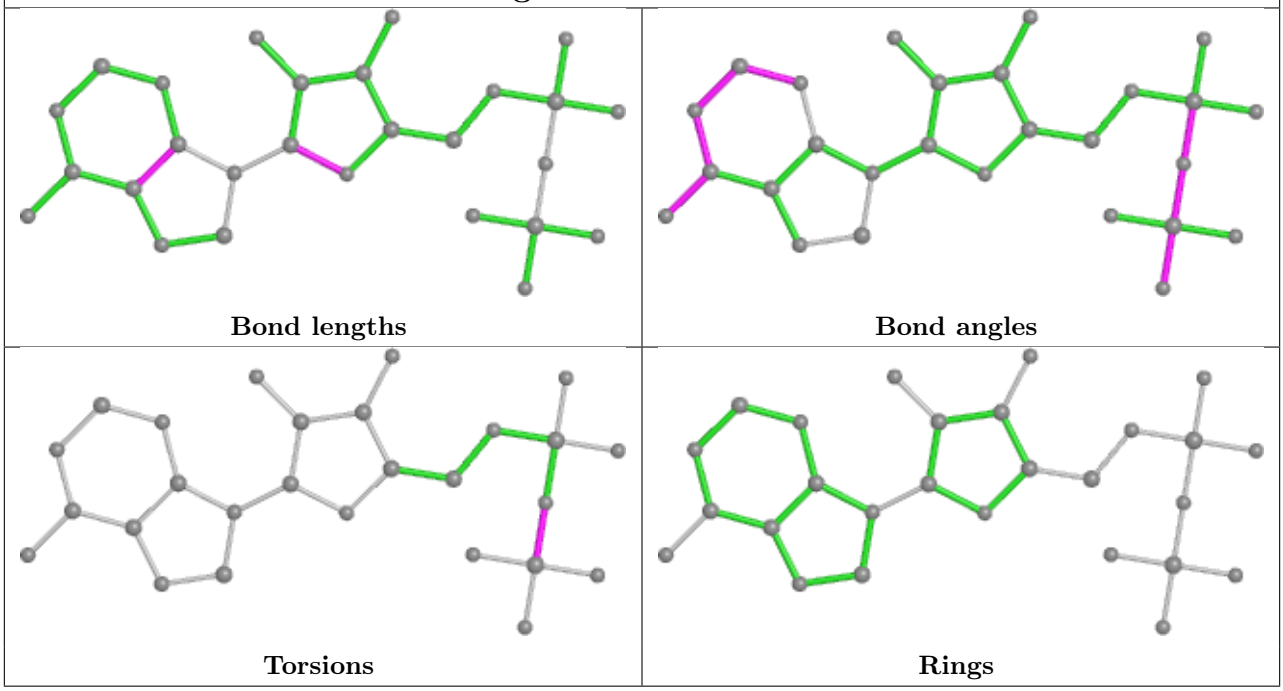
There are no ring outliers.

10 monomers are involved in 14 short contacts:

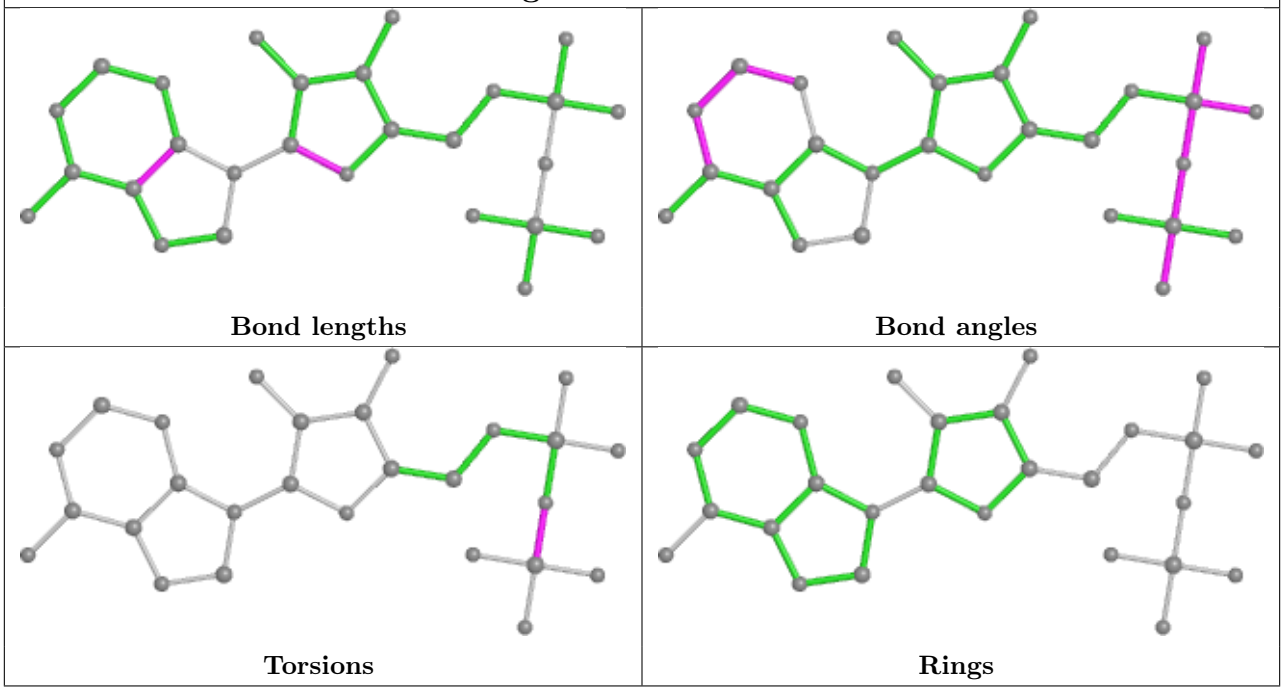
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	3502	ADP	2	0
6	D	502	ADP	1	0
6	A	2502	ADP	2	0
6	A	1502	ADP	2	0
6	A	502	ADP	2	0
6	D	4502	ADP	1	0
6	A	4502	ADP	1	0
6	D	2502	ADP	1	0
5	A	4501	ALF	1	0
6	D	1502	ADP	2	0

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.

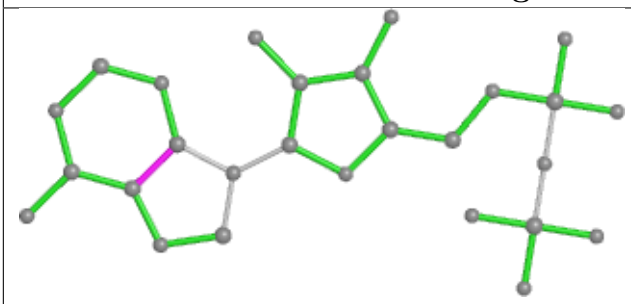
Ligand ADP D 3502



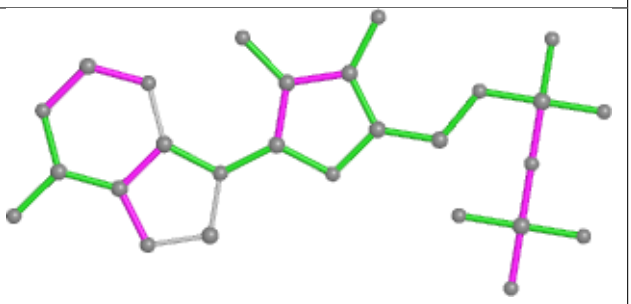
Ligand ADP D 502



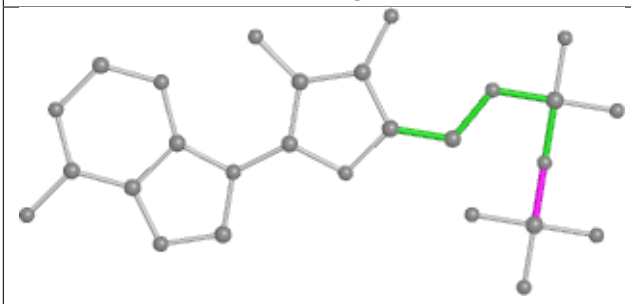
Ligand ADP A 2502



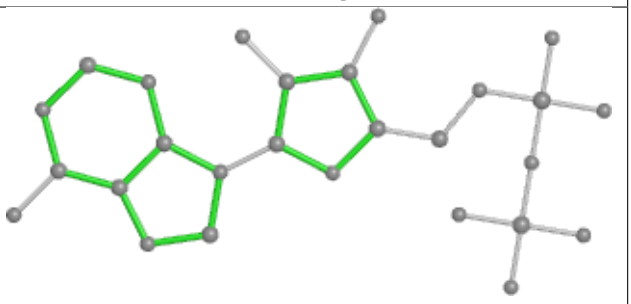
Bond lengths



Bond angles

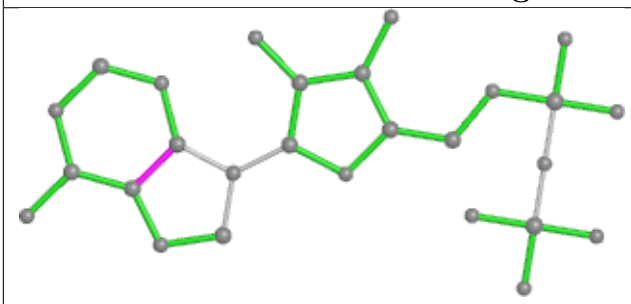


Torsions

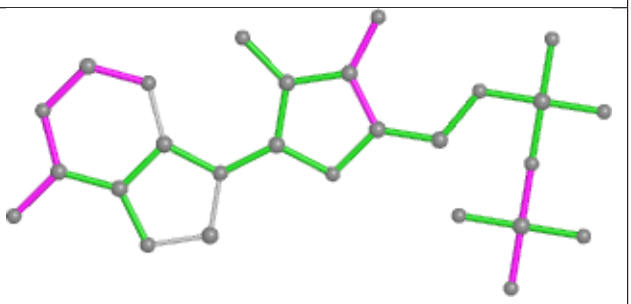


Rings

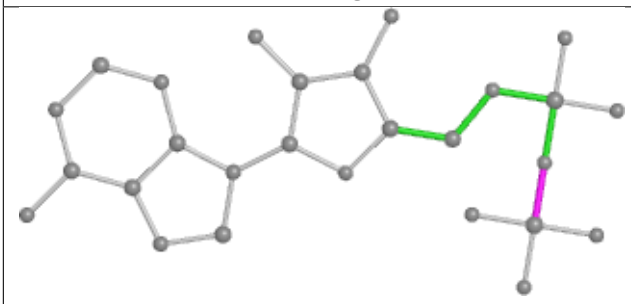
Ligand ADP A 1502



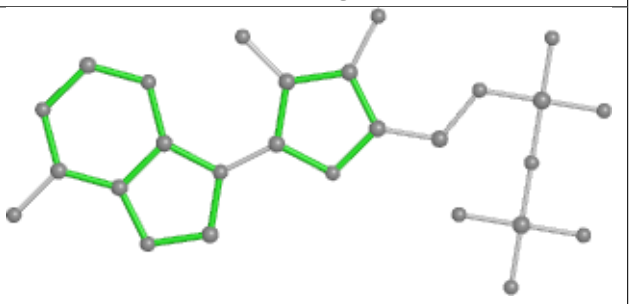
Bond lengths



Bond angles

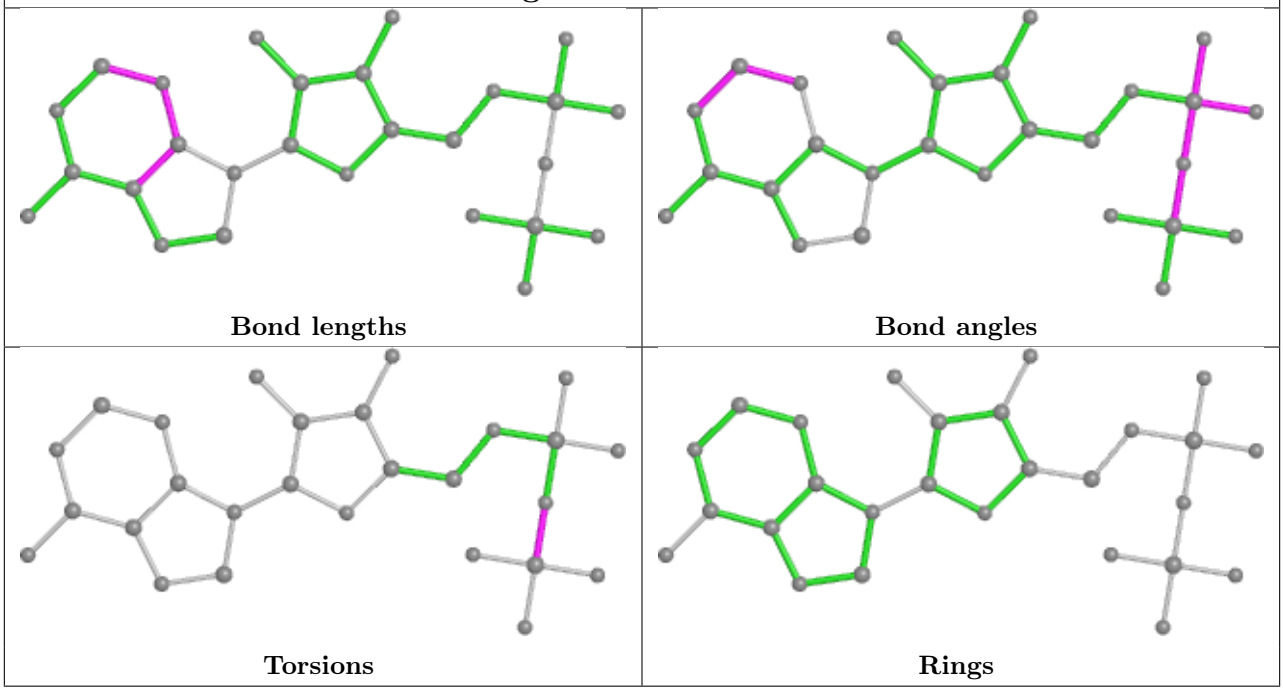


Torsions

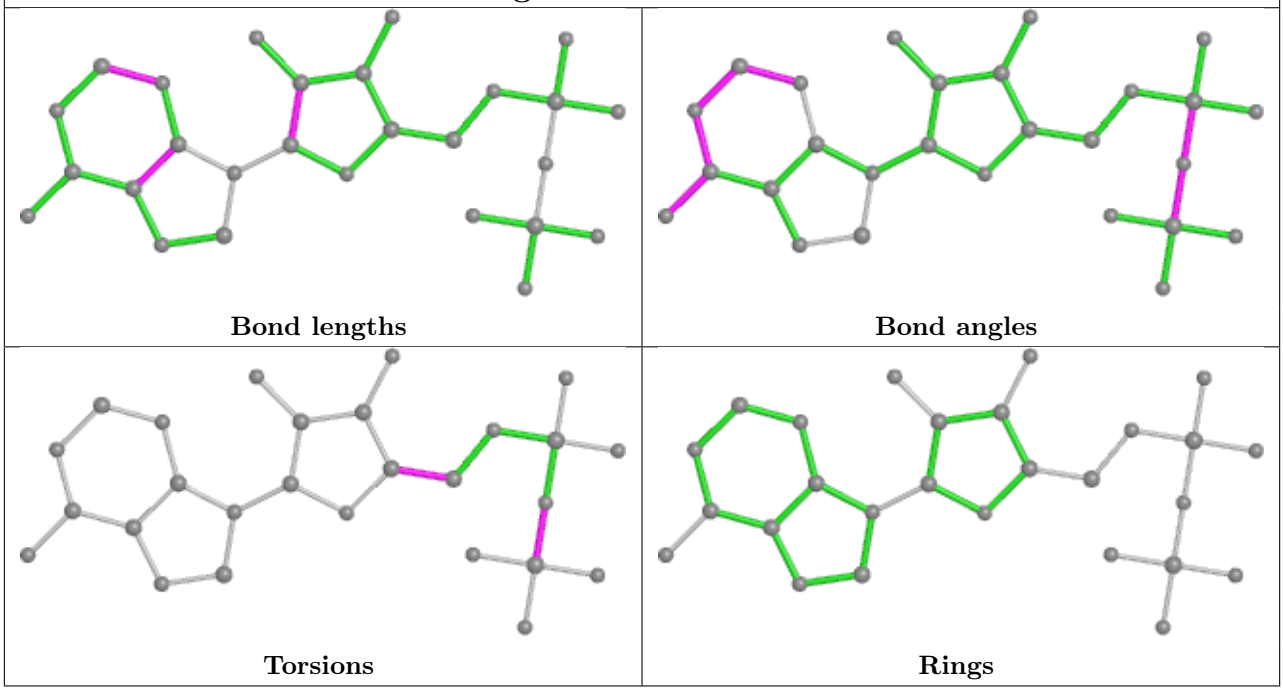


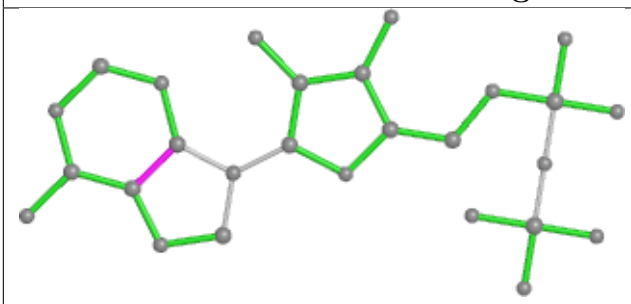
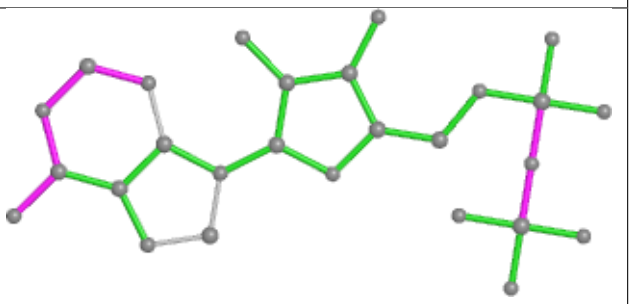
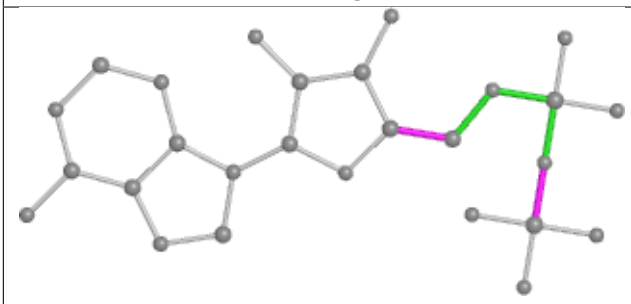
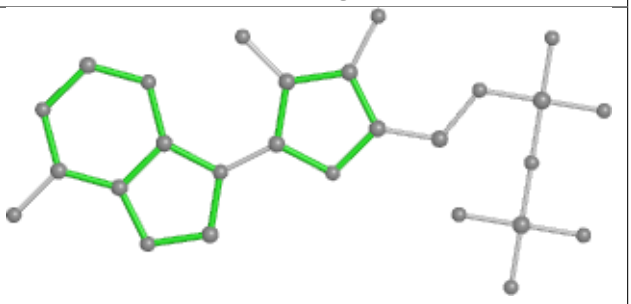
Rings

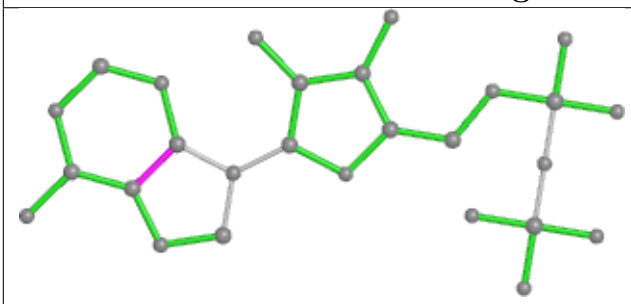
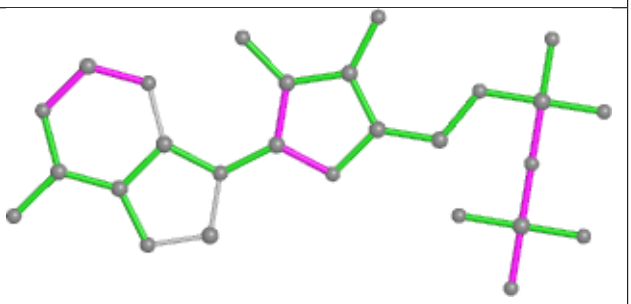
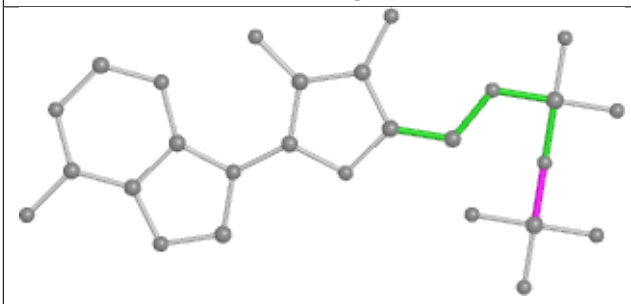
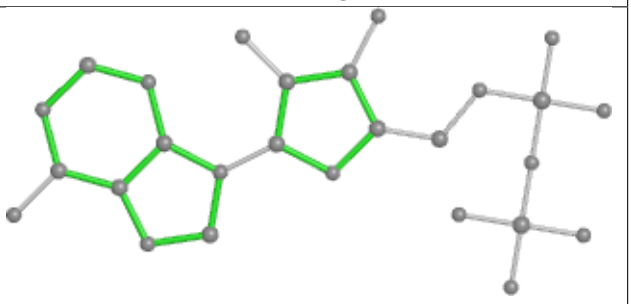
Ligand ADP A 502



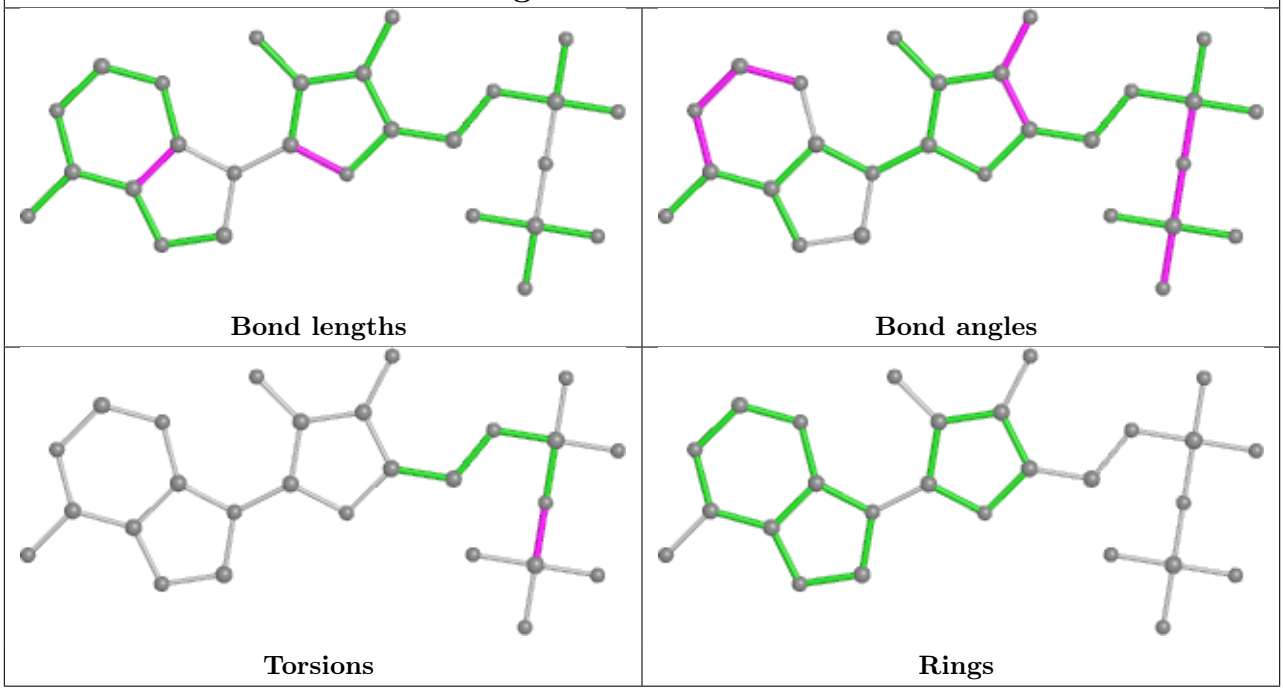
Ligand ADP D 4502



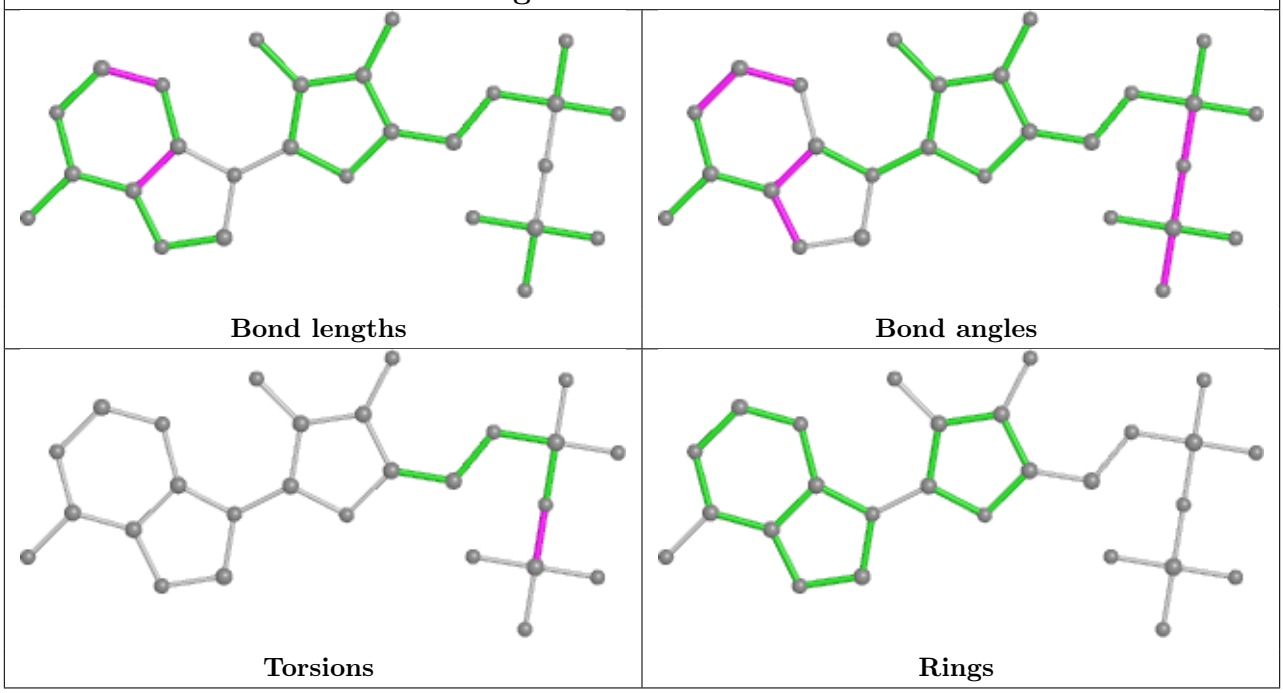
Ligand ADP A 4502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP A 3502	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP D 2502



Ligand ADP D 1502



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	13/15 (86%)	0.37	0	100	100	14, 20, 22, 24	0
1	E	13/15 (86%)	0.14	0	100	100	11, 19, 23, 28	0
2	C	11/12 (91%)	2.44	5 (45%)	0	0	46, 49, 51, 56	0
2	F	12/12 (100%)	3.35	11 (91%)	0	0	47, 49, 51, 51	0
3	A	1603/1706 (93%)	0.30	76 (4%)	31	31	19, 30, 45, 76	0
3	D	1603/1706 (93%)	0.21	53 (3%)	46	45	18, 30, 45, 75	0
All	All	3255/3466 (93%)	0.28	145 (4%)	33	33	11, 30, 48, 76	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	4316	ALA	6.1
2	F	2012	DA	6.0
3	D	4291	TYR	6.0
3	A	3001	ALA	5.6
2	F	2004	DA	5.2
2	C	2014	DA	5.1
3	D	4001	ALA	4.9
3	A	298	ILE	4.8
3	D	2001	ALA	4.7
3	D	4314	GLU	4.7
3	D	4311	ASP	4.6
2	F	2006	DA	4.5
2	C	2004	DA	4.5
2	F	2007	DA	4.4
2	C	2006	DA	4.3
3	A	2200	GLY	4.3
3	D	4313	PRO	4.3
3	A	2002	ILE	4.1
3	D	4315	THR	4.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	4317	LYS	4.0
3	D	4295	GLY	3.9
2	C	2005	DA	3.9
3	D	4309	LEU	3.9
3	A	251	ILE	3.9
3	D	2236	ASN	3.8
3	A	50	ALA	3.8
3	A	4205	ASN	3.7
2	F	2005	DA	3.7
3	A	287	ALA	3.7
3	A	53	ALA	3.6
3	D	4232	LYS	3.5
3	A	1289	ALA	3.5
3	A	204	GLY	3.5
3	D	3023	LYS	3.5
3	A	299	GLY	3.5
3	A	2023	LYS	3.5
3	D	4310	LYS	3.5
3	A	1203	PHE	3.4
3	D	4298	ILE	3.4
3	A	200	GLY	3.3
3	A	252	ALA	3.3
3	D	4278	GLY	3.2
3	D	4301	GLY	3.2
3	A	289	ALA	3.2
2	F	2008	DA	3.2
3	A	319	ILE	3.2
3	D	4282	LYS	3.2
3	A	1288	GLY	3.2
3	D	4296	GLU	3.2
3	A	288	GLY	3.1
3	D	4290	TRP	3.1
3	A	4196	ARG	3.1
3	A	265	GLY	3.1
3	D	4306	THR	3.1
3	D	3296	GLU	3.1
3	A	2001	ALA	3.0
3	D	4284	ILE	3.0
3	A	282	LYS	3.0
3	A	274	LEU	3.0
3	D	3295	GLY	2.9
3	D	2002	ILE	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	4297	LYS	2.9
3	A	4023	LYS	2.9
3	D	4287	ALA	2.9
3	A	3203	PHE	2.9
3	A	1130	ASP	2.9
3	D	4153	ALA	2.9
3	D	1313	PRO	2.9
3	A	307	ALA	2.9
3	D	3204	GLY	2.8
3	A	1202	MET	2.8
3	D	4136	GLY	2.8
3	A	2202	MET	2.8
3	D	4152	LYS	2.7
2	F	2011	DA	2.7
3	D	4154	GLU	2.7
3	A	253	ALA	2.7
3	D	4279	VAL	2.7
3	A	1021	PHE	2.7
3	D	4321	LYS	2.7
3	A	4001	ALA	2.7
3	A	2286	LYS	2.7
3	A	1204	GLY	2.7
3	A	1295	GLY	2.7
3	A	1305	ALA	2.7
3	D	137	ALA	2.6
3	D	4312	ASN	2.6
3	D	4294	LYS	2.6
3	A	4002	ILE	2.6
3	D	333	SER	2.6
3	D	4231	VAL	2.5
2	F	2014	DA	2.5
3	D	4318	GLU	2.5
3	A	308	TRP	2.5
3	D	3202	MET	2.5
3	A	3333	SER	2.5
2	F	2015	DA	2.5
3	A	3023	LYS	2.5
3	D	37	VAL	2.5
3	D	4236	ASN	2.5
3	A	3002	ILE	2.4
3	A	2287	ALA	2.4
3	A	3287	ALA	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
3	D	4205	ASN	2.4
3	A	296	GLU	2.4
3	A	2297	LYS	2.4
3	A	2201	VAL	2.4
3	A	276	ASP	2.4
3	A	1299	GLY	2.4
3	A	235	GLU	2.4
3	A	205	ASN	2.4
2	F	2013	DA	2.3
3	A	1001	ALA	2.3
2	C	2007	DA	2.3
3	A	2203	PHE	2.3
3	A	144	ASP	2.3
3	A	3234	GLY	2.2
3	D	1234	GLY	2.2
3	A	2003	ASP	2.2
3	A	300	GLN	2.2
3	D	2005	ASN	2.2
3	D	235	GLU	2.2
3	A	135	SER	2.2
3	A	330	ASN	2.2
3	D	2023	LYS	2.2
3	A	199	ILE	2.2
3	A	202	MET	2.2
3	D	2019	LYS	2.2
3	A	2025	SER	2.1
3	A	186	ASN	2.1
3	A	333	SER	2.1
3	A	4117	SER	2.1
2	F	2009	DA	2.1
3	D	4281	GLU	2.1
3	A	1298	ILE	2.1
3	D	1202	MET	2.1
3	A	2024	GLY	2.1
3	A	1291	TYR	2.1
3	A	203	PHE	2.1
3	A	331	PRO	2.1
3	A	4168	ALA	2.1
3	A	272	GLY	2.1
3	A	3202	MET	2.1
3	A	54	GLY	2.0
3	A	2113	ASN	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 monosaccharides 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	0.81	0.20	26,30,32,32	0
4	MG	D	4500	1/1	0.88	0.22	17,17,17,17	0
4	MG	A	4500	1/1	0.89	0.12	2,2,2,2	0
5	ALF	A	4501	5/5	0.92	0.15	36,38,40,40	0
6	ADP	A	502	27/27	0.92	0.26	18,21,27,29	0
6	ADP	A	4502	27/27	0.93	0.13	11,19,23,23	0
4	MG	D	1500	1/1	0.94	0.36	2,2,2,2	0
4	MG	A	1500	1/1	0.94	0.33	3,3,3,3	0
6	ADP	A	2502	27/27	0.95	0.21	2,2,2,5	0
5	ALF	A	2501	5/5	0.95	0.27	2,2,2,2	0
6	ADP	D	3502	27/27	0.95	0.18	2,4,9,9	0
6	ADP	D	4502	27/27	0.95	0.13	17,19,21,24	0
5	ALF	D	3501	5/5	0.96	0.21	2,2,3,6	0
6	ADP	A	3502	27/27	0.96	0.18	2,2,2,2	0
4	MG	A	2500	1/1	0.96	0.36	2,2,2,2	0
6	ADP	D	2502	27/27	0.96	0.19	2,5,6,7	0
4	MG	A	500	1/1	0.96	0.56	24,24,24,24	0
6	ADP	A	1502	27/27	0.96	0.23	2,2,3,5	0
5	ALF	A	501	5/5	0.97	0.34	17,21,22,23	0
6	ADP	D	502	27/27	0.97	0.20	2,2,4,5	0
6	ADP	D	1502	27/27	0.97	0.20	2,2,3,5	0
5	ALF	D	1501	5/5	0.97	0.27	2,2,2,2	0
4	MG	D	2500	1/1	0.97	0.35	2,2,2,2	0
5	ALF	A	3501	5/5	0.97	0.26	2,2,2,2	0
5	ALF	D	501	5/5	0.98	0.29	2,2,2,2	0
4	MG	A	3500	1/1	0.98	0.37	2,2,2,2	0
5	ALF	D	2501	5/5	0.98	0.33	2,2,2,2	0

Continued on next page...

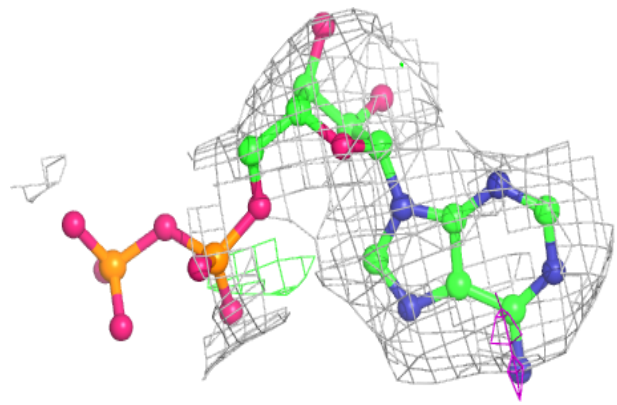
Continued from previous page...

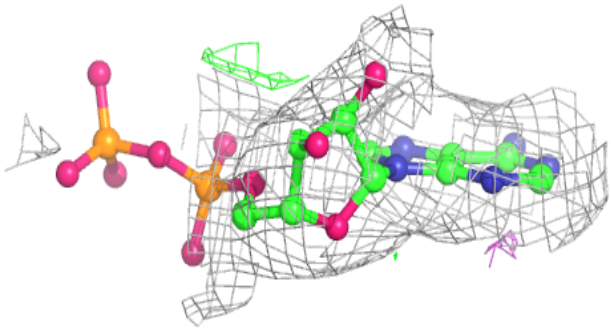
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	MG	D	3500	1/1	0.98	0.28	6,6,6,6	0
5	ALF	A	1501	5/5	0.98	0.29	2,2,4,5	0
4	MG	D	500	1/1	0.99	0.23	5,5,5,5	0

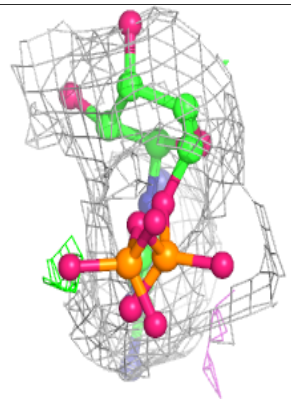
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 502:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)

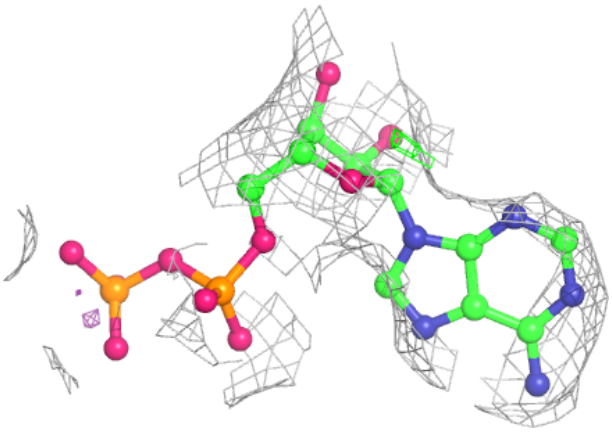


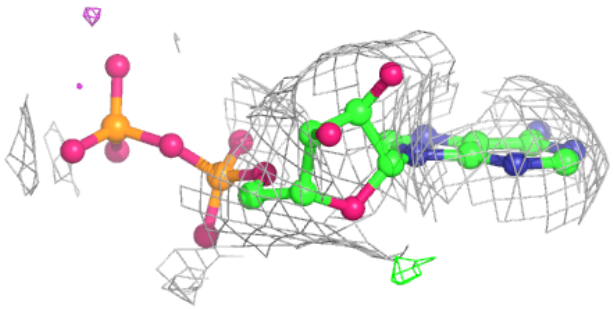




Electron density around ADP A 4502:

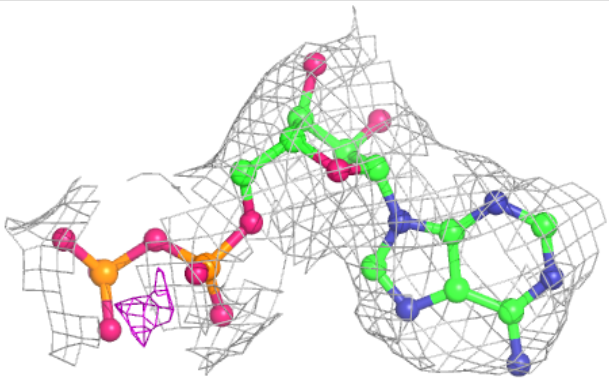
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

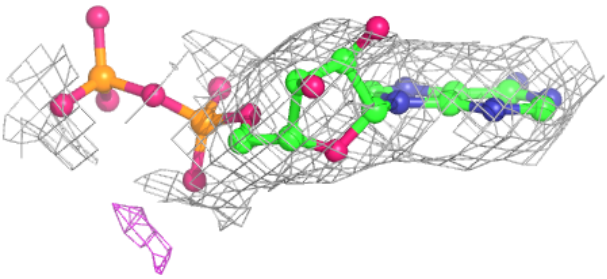


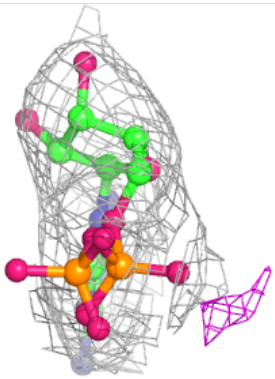


Electron density around ADP A 2502:

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

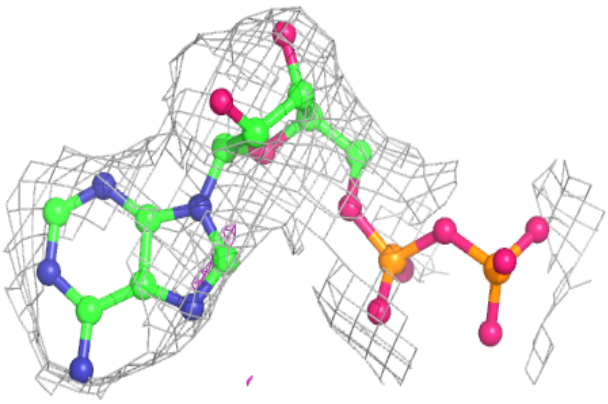


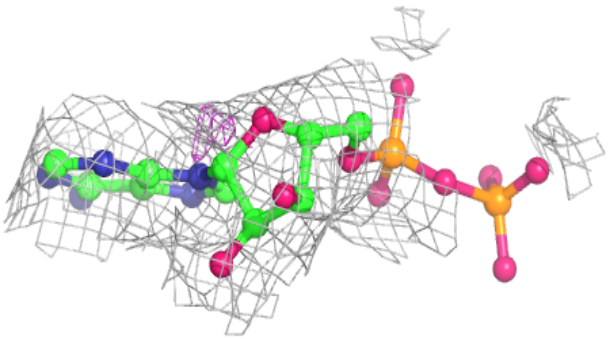


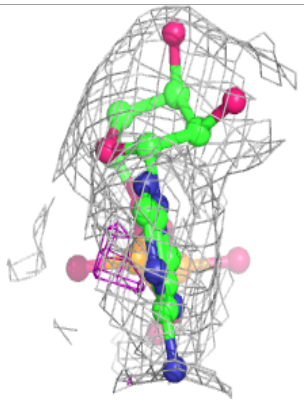


Electron density around ADP D 3502:

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

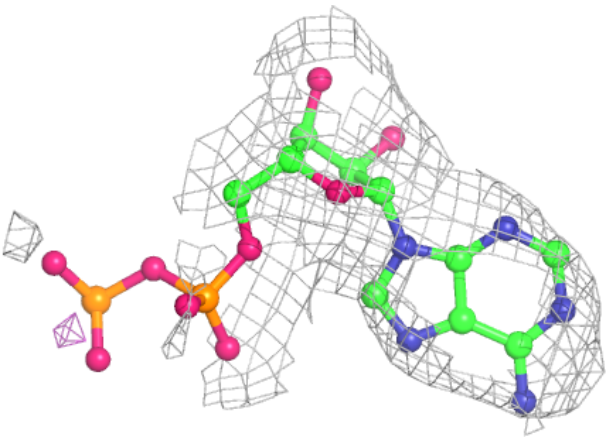


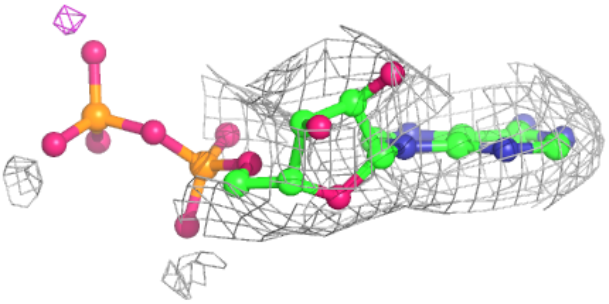


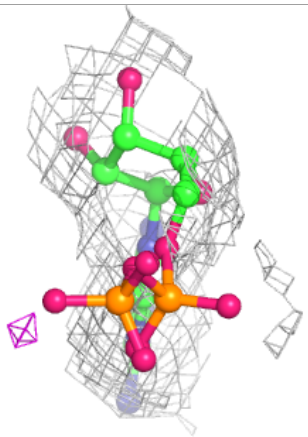


Electron density around ADP D 4502:

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

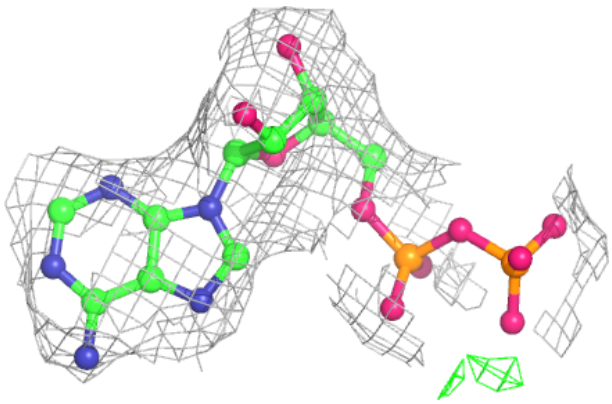


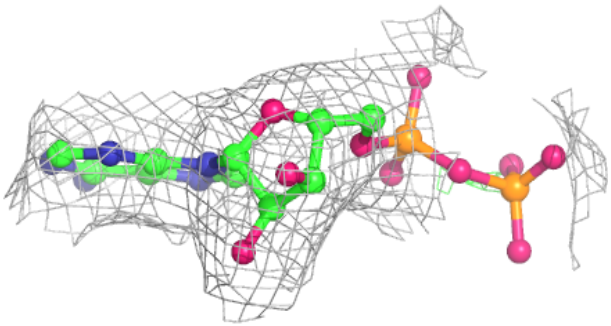


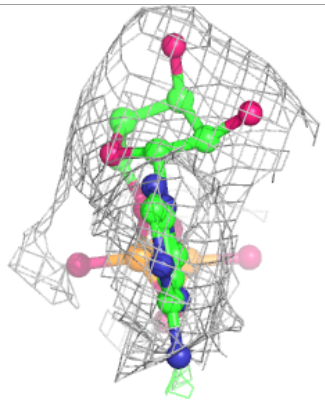


Electron density around ADP A 3502:

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

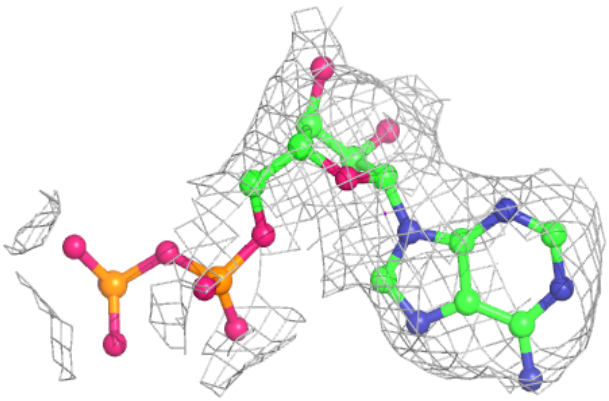


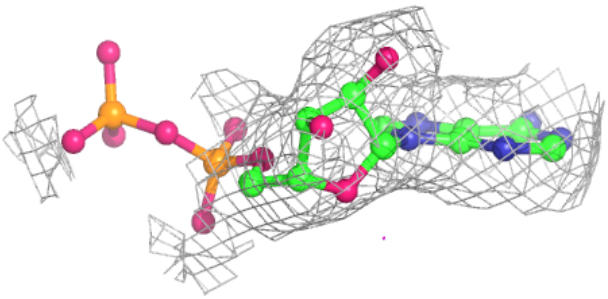


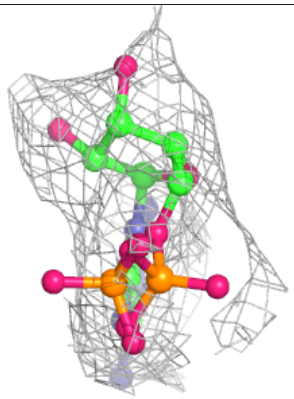


Electron density around ADP D 2502:

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

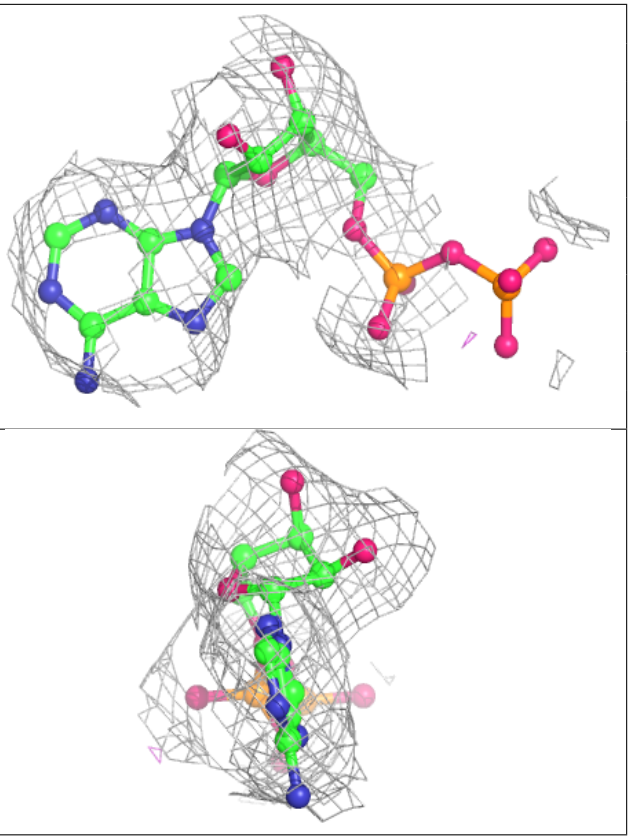






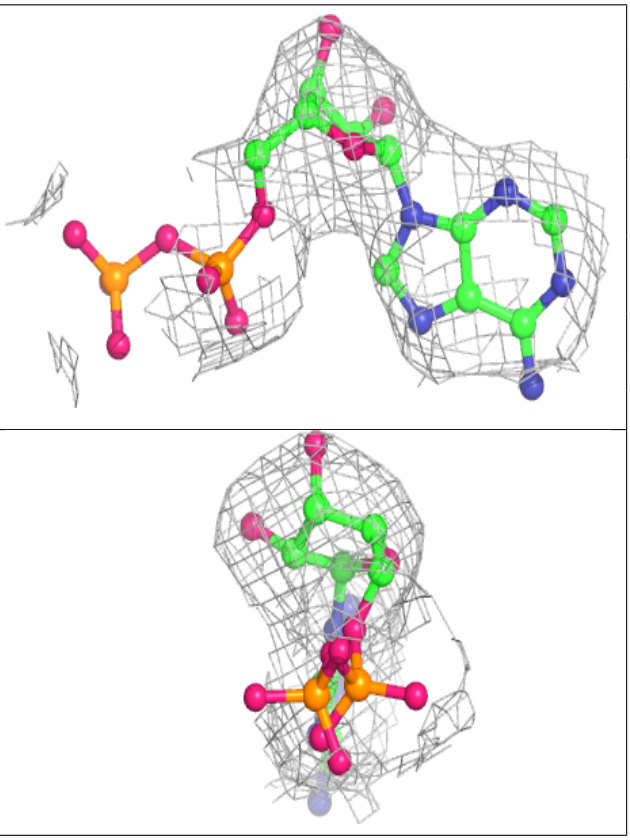
Electron density around ADP A 1502:

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



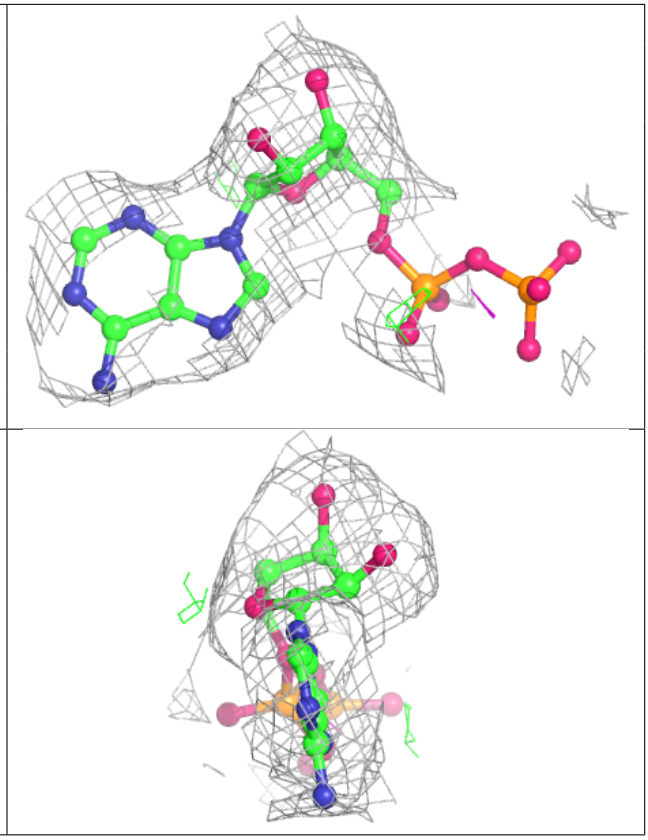
Electron density around ADP D 502:

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



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)



6.5 Other polymers (i)

There are no such residues in this entry.