W O R L D W I D E
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Dec 9, 2020 – 08:21 pm GMT

PDB ID	:	7AUD
Title	:	Structure of an engineered helicase domain construct for human Bloom syndrome protein (BLM)
Authors	:	Chen, X.; Oliver, A.W.
Deposited on	:	2020-11-02
Resolution	:	2.96 Å(reported)

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

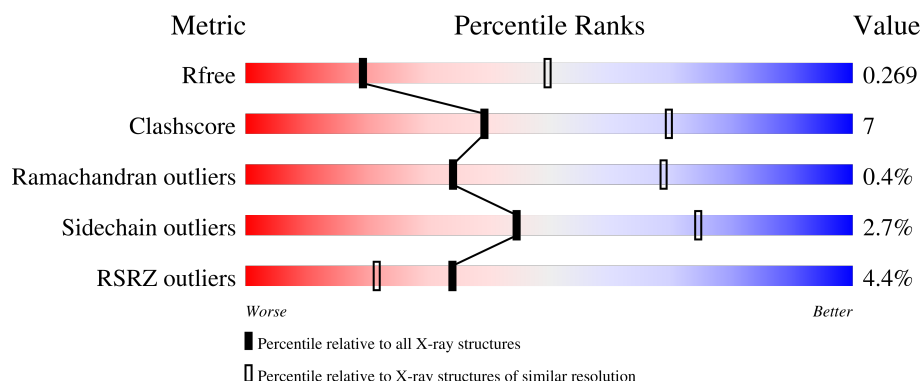|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.15.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.15.1

1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 2.96 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	Percentile Ranks	Value
Rfree		0.269
Clashscore		7
Ramachandran outliers		0.4%
Sidechain outliers		2.7%
RSRZ outliers		4.4%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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	A	563	3% / 74% / 18% · 7%
1	B	563	2% / 75% / 16% · 9%
1	C	563	2% / 71% / 19% · 9%
1	D	563	4% / 74% / 16% / 9%
1	E	563	4% / 75% / 15% · 9%

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Mol	Chain	Length	Quality of chain
1	F	563	8% / 74% / 17% / 8%
2	M	15	47% / 40% / 13%
2	N	15	53% / 33% / 13%
2	O	15	80% / 7% / 13%
2	P	15	87% / 13%
2	Q	15	60% / 27% / 13%
2	R	15	67% / 20% / 13%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 25271 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 protein called Bloom syndrome protein,Bloom syndrome protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	522	Total 4023	C 2551	N 703	O 737	S 32	1	2	0
1	B	513	Total 3890	C 2477	N 670	O 712	S 31	1	0	0
1	C	513	Total 3908	C 2483	N 683	O 710	S 32	1	1	0
1	D	510	Total 3792	C 2411	N 657	O 692	S 32	4	1	0
1	E	513	Total 3825	C 2427	N 665	O 703	S 30	2	1	0
1	F	516	Total 3750	C 2384	N 645	O 693	S 28	4	1	0

There are 186 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	610	MET	-	initiating methionine	UNP P54132
A	611	GLY	-	expression tag	UNP P54132
A	612	SER	-	expression tag	UNP P54132
A	613	ALA	-	expression tag	UNP P54132
A	614	TRP	-	expression tag	UNP P54132
A	615	SER	-	expression tag	UNP P54132
A	616	HIS	-	expression tag	UNP P54132
A	617	PRO	-	expression tag	UNP P54132
A	618	GLN	-	expression tag	UNP P54132
A	619	PHE	-	expression tag	UNP P54132
A	620	GLU	-	expression tag	UNP P54132
A	621	LYS	-	expression tag	UNP P54132
A	622	SER	-	expression tag	UNP P54132
A	623	SER	-	expression tag	UNP P54132
A	624	GLY	-	expression tag	UNP P54132
A	625	LEU	-	expression tag	UNP P54132
A	626	GLU	-	expression tag	UNP P54132

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Chain	Residue	Modelled	Actual	Comment	Reference
A	627	VAL	-	expression tag	UNP P54132
A	628	LEU	-	expression tag	UNP P54132
A	629	PHE	-	expression tag	UNP P54132
A	630	GLN	-	expression tag	UNP P54132
A	631	GLY	-	expression tag	UNP P54132
A	632	GLY	-	expression tag	UNP P54132
A	633	PRO	-	expression tag	UNP P54132
A	634	HIS	-	expression tag	UNP P54132
A	635	MET	-	expression tag	UNP P54132
A	1197	GLY	-	linker	UNP P54132
A	1198	SER	-	linker	UNP P54132
A	1199	GLY	-	linker	UNP P54132
A	1200	GLY	-	linker	UNP P54132
A	1201	SER	-	linker	UNP P54132
B	610	MET	-	initiating methionine	UNP P54132
B	611	GLY	-	expression tag	UNP P54132
B	612	SER	-	expression tag	UNP P54132
B	613	ALA	-	expression tag	UNP P54132
B	614	TRP	-	expression tag	UNP P54132
B	615	SER	-	expression tag	UNP P54132
B	616	HIS	-	expression tag	UNP P54132
B	617	PRO	-	expression tag	UNP P54132
B	618	GLN	-	expression tag	UNP P54132
B	619	PHE	-	expression tag	UNP P54132
B	620	GLU	-	expression tag	UNP P54132
B	621	LYS	-	expression tag	UNP P54132
B	622	SER	-	expression tag	UNP P54132
B	623	SER	-	expression tag	UNP P54132
B	624	GLY	-	expression tag	UNP P54132
B	625	LEU	-	expression tag	UNP P54132
B	626	GLU	-	expression tag	UNP P54132
B	627	VAL	-	expression tag	UNP P54132
B	628	LEU	-	expression tag	UNP P54132
B	629	PHE	-	expression tag	UNP P54132
B	630	GLN	-	expression tag	UNP P54132
B	631	GLY	-	expression tag	UNP P54132
B	632	GLY	-	expression tag	UNP P54132
B	633	PRO	-	expression tag	UNP P54132
B	634	HIS	-	expression tag	UNP P54132
B	635	MET	-	expression tag	UNP P54132
B	1197	GLY	-	linker	UNP P54132
B	1198	SER	-	linker	UNP P54132

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Chain	Residue	Modelled	Actual	Comment	Reference
B	1199	GLY	-	linker	UNP P54132
B	1200	GLY	-	linker	UNP P54132
B	1201	SER	-	linker	UNP P54132
C	610	MET	-	initiating methionine	UNP P54132
C	611	GLY	-	expression tag	UNP P54132
C	612	SER	-	expression tag	UNP P54132
C	613	ALA	-	expression tag	UNP P54132
C	614	TRP	-	expression tag	UNP P54132
C	615	SER	-	expression tag	UNP P54132
C	616	HIS	-	expression tag	UNP P54132
C	617	PRO	-	expression tag	UNP P54132
C	618	GLN	-	expression tag	UNP P54132
C	619	PHE	-	expression tag	UNP P54132
C	620	GLU	-	expression tag	UNP P54132
C	621	LYS	-	expression tag	UNP P54132
C	622	SER	-	expression tag	UNP P54132
C	623	SER	-	expression tag	UNP P54132
C	624	GLY	-	expression tag	UNP P54132
C	625	LEU	-	expression tag	UNP P54132
C	626	GLU	-	expression tag	UNP P54132
C	627	VAL	-	expression tag	UNP P54132
C	628	LEU	-	expression tag	UNP P54132
C	629	PHE	-	expression tag	UNP P54132
C	630	GLN	-	expression tag	UNP P54132
C	631	GLY	-	expression tag	UNP P54132
C	632	GLY	-	expression tag	UNP P54132
C	633	PRO	-	expression tag	UNP P54132
C	634	HIS	-	expression tag	UNP P54132
C	635	MET	-	expression tag	UNP P54132
C	1197	GLY	-	linker	UNP P54132
C	1198	SER	-	linker	UNP P54132
C	1199	GLY	-	linker	UNP P54132
C	1200	GLY	-	linker	UNP P54132
C	1201	SER	-	linker	UNP P54132
D	610	MET	-	initiating methionine	UNP P54132
D	611	GLY	-	expression tag	UNP P54132
D	612	SER	-	expression tag	UNP P54132
D	613	ALA	-	expression tag	UNP P54132
D	614	TRP	-	expression tag	UNP P54132
D	615	SER	-	expression tag	UNP P54132
D	616	HIS	-	expression tag	UNP P54132
D	617	PRO	-	expression tag	UNP P54132

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Chain	Residue	Modelled	Actual	Comment	Reference
D	618	GLN	-	expression tag	UNP P54132
D	619	PHE	-	expression tag	UNP P54132
D	620	GLU	-	expression tag	UNP P54132
D	621	LYS	-	expression tag	UNP P54132
D	622	SER	-	expression tag	UNP P54132
D	623	SER	-	expression tag	UNP P54132
D	624	GLY	-	expression tag	UNP P54132
D	625	LEU	-	expression tag	UNP P54132
D	626	GLU	-	expression tag	UNP P54132
D	627	VAL	-	expression tag	UNP P54132
D	628	LEU	-	expression tag	UNP P54132
D	629	PHE	-	expression tag	UNP P54132
D	630	GLN	-	expression tag	UNP P54132
D	631	GLY	-	expression tag	UNP P54132
D	632	GLY	-	expression tag	UNP P54132
D	633	PRO	-	expression tag	UNP P54132
D	634	HIS	-	expression tag	UNP P54132
D	635	MET	-	expression tag	UNP P54132
D	1197	GLY	-	linker	UNP P54132
D	1198	SER	-	linker	UNP P54132
D	1199	GLY	-	linker	UNP P54132
D	1200	GLY	-	linker	UNP P54132
D	1201	SER	-	linker	UNP P54132
E	610	MET	-	initiating methionine	UNP P54132
E	611	GLY	-	expression tag	UNP P54132
E	612	SER	-	expression tag	UNP P54132
E	613	ALA	-	expression tag	UNP P54132
E	614	TRP	-	expression tag	UNP P54132
E	615	SER	-	expression tag	UNP P54132
E	616	HIS	-	expression tag	UNP P54132
E	617	PRO	-	expression tag	UNP P54132
E	618	GLN	-	expression tag	UNP P54132
E	619	PHE	-	expression tag	UNP P54132
E	620	GLU	-	expression tag	UNP P54132
E	621	LYS	-	expression tag	UNP P54132
E	622	SER	-	expression tag	UNP P54132
E	623	SER	-	expression tag	UNP P54132
E	624	GLY	-	expression tag	UNP P54132
E	625	LEU	-	expression tag	UNP P54132
E	626	GLU	-	expression tag	UNP P54132
E	627	VAL	-	expression tag	UNP P54132
E	628	LEU	-	expression tag	UNP P54132

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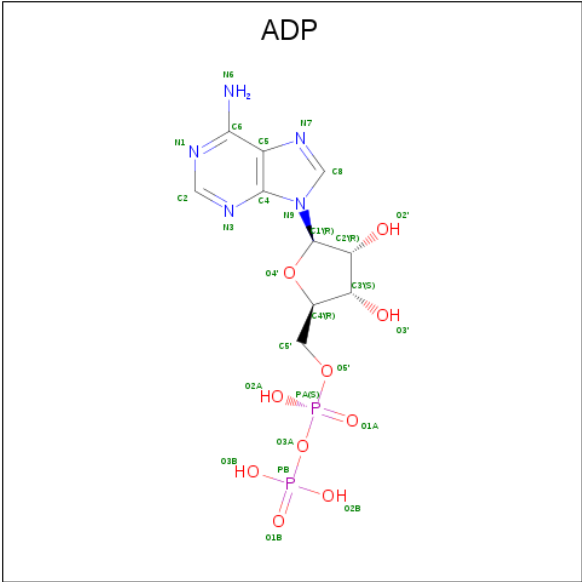| Chain	Residue	Modelled	Actual	Comment	Reference
E	629	PHE	-	expression tag	UNP P54132
E	630	GLN	-	expression tag	UNP P54132
E	631	GLY	-	expression tag	UNP P54132
E	632	GLY	-	expression tag	UNP P54132
E	633	PRO	-	expression tag	UNP P54132
E	634	HIS	-	expression tag	UNP P54132
E	635	MET	-	expression tag	UNP P54132
E	1197	GLY	-	linker	UNP P54132
E	1198	SER	-	linker	UNP P54132
E	1199	GLY	-	linker	UNP P54132
E	1200	GLY	-	linker	UNP P54132
E	1201	SER	-	linker	UNP P54132
F	610	MET	-	initiating methionine	UNP P54132
F	611	GLY	-	expression tag	UNP P54132
F	612	SER	-	expression tag	UNP P54132
F	613	ALA	-	expression tag	UNP P54132
F	614	TRP	-	expression tag	UNP P54132
F	615	SER	-	expression tag	UNP P54132
F	616	HIS	-	expression tag	UNP P54132
F	617	PRO	-	expression tag	UNP P54132
F	618	GLN	-	expression tag	UNP P54132
F	619	PHE	-	expression tag	UNP P54132
F	620	GLU	-	expression tag	UNP P54132
F	621	LYS	-	expression tag	UNP P54132
F	622	SER	-	expression tag	UNP P54132
F	623	SER	-	expression tag	UNP P54132
F	624	GLY	-	expression tag	UNP P54132
F	625	LEU	-	expression tag	UNP P54132
F	626	GLU	-	expression tag	UNP P54132
F	627	VAL	-	expression tag	UNP P54132
F	628	LEU	-	expression tag	UNP P54132
F	629	PHE	-	expression tag	UNP P54132
F	630	GLN	-	expression tag	UNP P54132
F	631	GLY	-	expression tag	UNP P54132
F	632	GLY	-	expression tag	UNP P54132
F	633	PRO	-	expression tag	UNP P54132
F	634	HIS	-	expression tag	UNP P54132
F	635	MET	-	expression tag	UNP P54132
F	1197	GLY	-	linker	UNP P54132
F	1198	SER	-	linker	UNP P54132
F	1199	GLY	-	linker	UNP P54132
F	1200	GLY	-	linker	UNP P54132

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1201	SER	-	linker	UNP P54132

- Molecule 2 is a DNA chain called DNA (5'-D(*GP*TP*AP*CP*CP*CP*GP*AP*TP*GP* TP*GP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	M	13	Total	C	N	O	P	0	0	0
			264	127	47	78	12			
2	N	13	Total	C	N	O	P	0	0	0
			264	127	47	78	12			
2	O	13	Total	C	N	O	P	0	0	0
			264	127	47	78	12			
2	P	13	Total	C	N	O	P	0	0	0
			267	127	47	80	13			
2	Q	13	Total	C	N	O	P	0	0	0
			267	127	47	80	13			
2	R	13	Total	C	N	O	P	0	0	0
			264	127	47	78	12			

- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

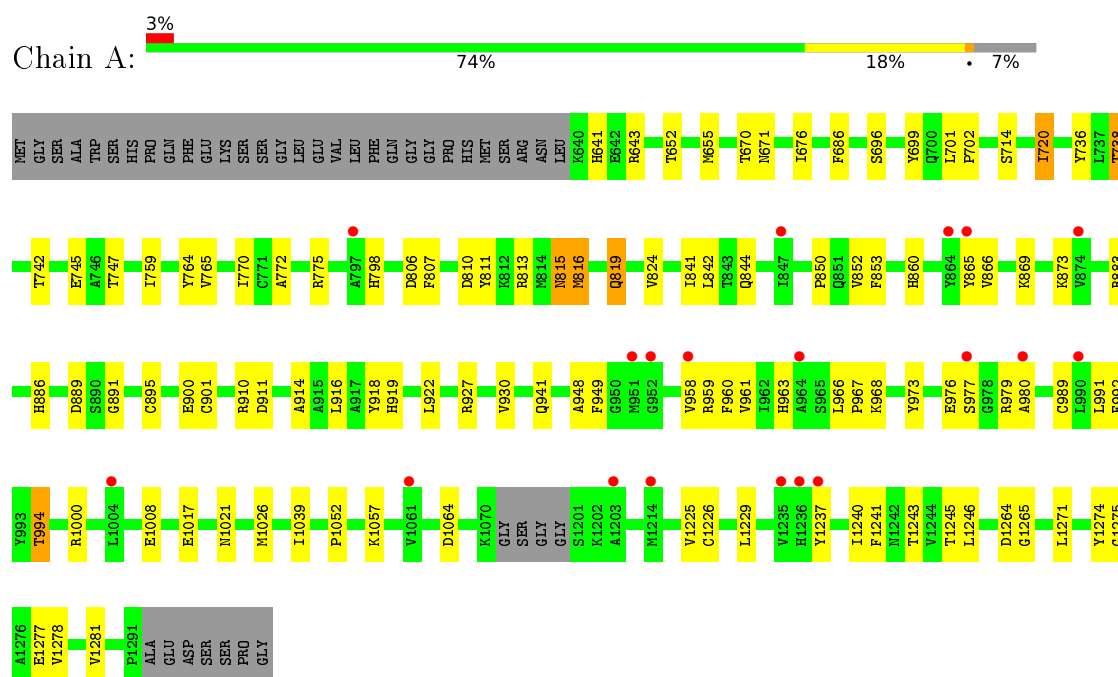| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	1	Total	Zn	0	0
			1	1		
3	E	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		
3	A	1	Total	Zn	0	0
			1	1		
3	F	1	Total	Zn	0	0
			1	1		

- Molecule 4 is A D E N O S I N E - 5'- D I P H O S P H A T E (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

ADP

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	F	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 5 is N-(2,3-dimethyl-5-sulfamoylphenyl)-4-(2-methylthiazol-4-yl)benzamide (three-letter code: RY8) (formula: $C_{19}H_{19}N_3O_3S_2$) (labeled as "Ligand of Interest" by depositor).

RY8
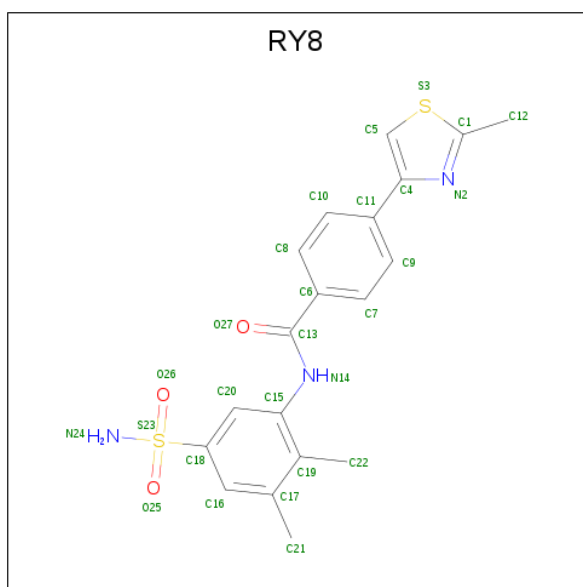
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 27	C 19	N 3	O 3	S 2	0	0
5	B	1	Total 27	C 19	N 3	O 3	S 2	0	0
5	C	1	Total 27	C 19	N 3	O 3	S 2	0	0
5	D	1	Total 27	C 19	N 3	O 3	S 2	0	0
5	E	1	Total 27	C 19	N 3	O 3	S 2	0	0
5	F	1	Total 27	C 19	N 3	O 3	S 2	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).

PG4

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		
6	A	1	Total	C	O	0	0
			13	8	5		
6	B	1	Total	C	O	0	0
			13	8	5		
6	C	1	Total	C	O	0	0
			13	8	5		
6	C	1	Total	C	O	0	0
			13	8	5		
6	D	1	Total	C	O	0	0
			13	8	5		
6	E	1	Total	C	O	0	0
			13	8	5		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	P	1	Total	Mg	0	0
			1	1		
7	Q	2	Total	Mg	0	0
			2	2		
7	N	1	Total	Mg	0	0
			1	1		
7	F	1	Total	Mg	0	0
			1	1		
7	M	1	Total	Mg	0	0
			1	1		

• Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	31	Total 31	O 31	0	0
8	B	16	Total 16	O 16	0	0
8	C	5	Total 5	O 5	0	0
8	D	4	Total 4	O 4	0	0
8	E	6	Total 6	O 6	0	0
8	F	1	Total 1	O 1	0	0
8	M	1	Total 1	O 1	0	0
8	Q	2	Total 2	O 2	0	0

3 Residue-property plots ⓘ

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: Bloom syndrome protein,Bloom syndrome protein

- Molecule 1: Bloom syndrome protein,Bloom syndrome protein

● Molecule 1: Bloom syndrome protein,Bloom syndrome protein

Chain C:

● Molecule 1: Bloom syndrome protein,Bloom syndrome protein

Chain D:

● Molecule 1: Bloom syndrome protein,Bloom syndrome protein

Chain E:
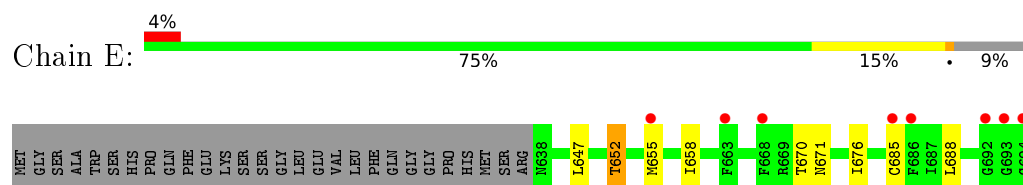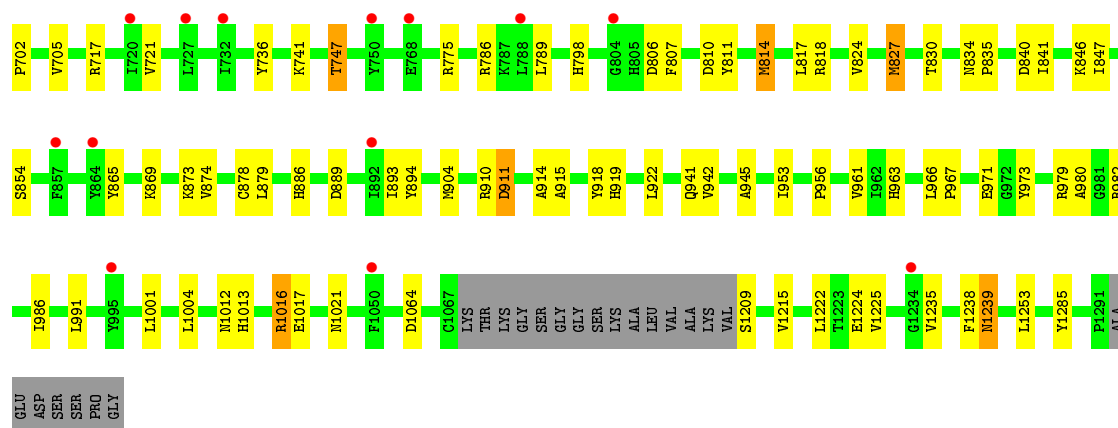
• Molecule 1: Bloom syndrome protein,Bloom syndrome protein
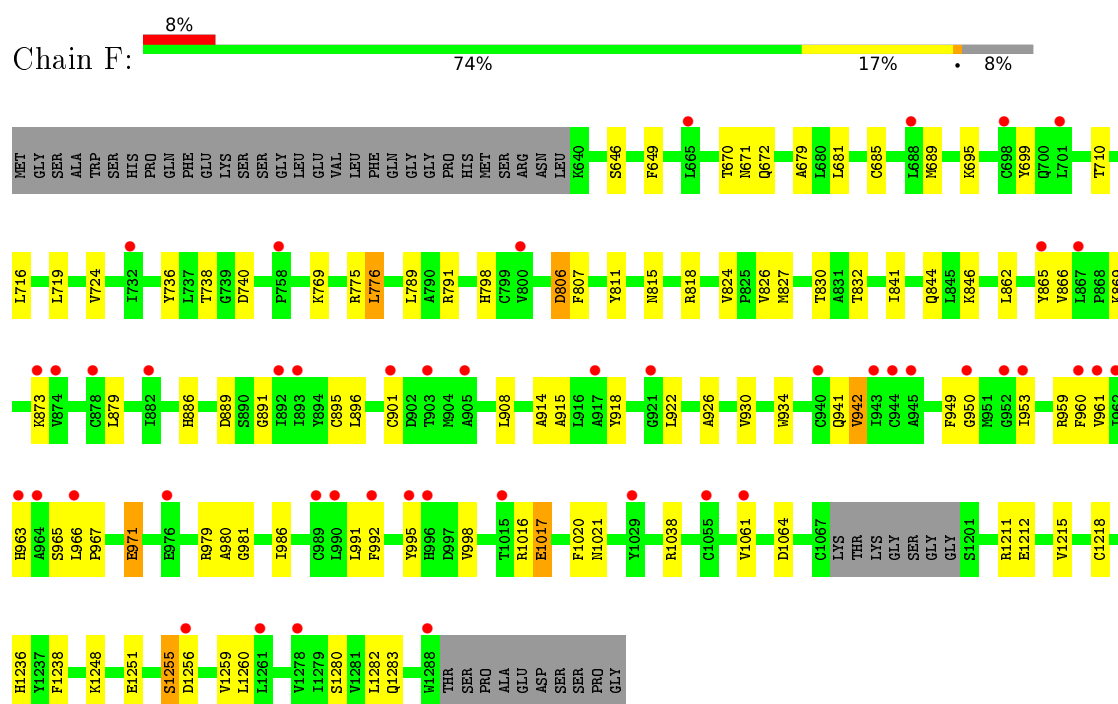
Chain F:

• Molecule 2: DNA (5'-D(*GP*TP*AP*CP*CP*CP*GP*AP*TP*GP*TP*GP*T)-3')

Chain M:

• Molecule 2: DNA (5'-D(*GP*TP*AP*CP*CP*CP*GP*AP*TP*GP*TP*GP*T)-3')

Chain N:

• Molecule 2: DNA (5'-D(*GP*TP*AP*CP*CP*CP*GP*AP*TP*GP*TP*GP*T)-3')

Chain O:

• Molecule 2: DNA (5'-D(*GP*TP*AP*CP*CP*CP*GP*AP*TP*GP*TP*GP*T)-3')

Chain P:

• Molecule 2: DNA (5'-D(*GP*TP*AP*CP*CP*CP*GP*AP*TP*GP*TP*GP*T)-3')

Chain Q:

• Molecule 2: DNA (5'-D(*GP*TP*AP*CP*CP*CP*GP*AP*TP*GP*TP*GP*T)-3')

Chain R:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	84.92Å 111.71Å 132.34Å 72.64° 80.18° 79.22°	Depositor
Resolution (Å)	47.28 – 2.96 125.37 – 2.96	Depositor EDS
% Data completeness (in resolution range)	97.6 (47.28-2.96) 92.2 (125.37-2.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.14 (at 2.96Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.229 , 0.269 0.229 , 0.269	Depositor DCC
R_{free} test set	4642 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	69.9	Xtriage
Anisotropy	0.428	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 62.6	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	25271	wwPDB-VP
Average B, all atoms (Å^2)	92.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: PG4, MG, RY8, ZN, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$>5	RMSZ	#$|Z|$>5
1	A	0.25	0/4117	0.43	0/5590
1	B	0.25	0/3978	0.43	0/5415
1	C	0.26	0/3999	0.45	0/5439
1	D	0.25	0/3882	0.44	0/5290
1	E	0.25	0/3915	0.44	0/5338
1	F	0.27	0/3838	0.45	0/5247
2	M	0.56	0/295	0.94	0/454
2	N	0.54	0/295	0.96	0/454
2	O	0.57	0/295	0.98	0/454
2	P	0.54	0/298	0.96	0/458
2	Q	0.54	0/298	0.96	0/458
2	R	0.56	0/295	0.95	0/454
All	All	0.28	0/25505	0.50	0/35051

There are no bond length outliers.

There are no bond angle outliers.

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	A	4023	0	3844	64	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3890	0	3651	53	0
1	C	3908	0	3689	67	0
1	D	3792	0	3481	55	0
1	E	3825	0	3517	48	0
1	F	3750	0	3370	60	0
2	M	264	0	149	7	0
2	N	264	0	149	4	0
2	O	264	0	149	1	0
2	P	267	0	148	0	0
2	Q	267	0	148	3	0
2	R	264	0	149	3	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	1	0
4	D	27	0	12	0	0
4	E	27	0	12	0	0
4	F	27	0	12	1	0
5	A	27	0	0	0	0
5	B	27	0	0	0	0
5	C	27	0	0	0	0
5	D	27	0	0	1	0
5	E	27	0	0	2	0
5	F	27	0	0	0	0
6	A	26	0	36	2	0
6	B	13	0	18	1	0
6	C	26	0	36	2	0
6	D	13	0	18	1	0
6	E	13	0	18	0	0
7	F	1	0	0	0	0
7	M	1	0	0	0	0
7	N	1	0	0	0	0
7	P	1	0	0	0	0
7	Q	2	0	0	0	0
8	A	31	0	0	0	0
8	B	16	0	0	0	0
8	C	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	4	0	0	0	0
8	E	6	0	0	0	0
8	F	1	0	0	0	0
8	M	1	0	0	0	0
8	Q	2	0	0	0	0
All	All	25271	0	22642	352	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 7.

The worst 5 of 352 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:669:ARG:H	1:C:672:GLN:HE21	1.25	0.83
1:A:1225:VAL:HG21	1:A:1281:VAL:HG11	1.59	0.83
1:C:737:LEU:HD13	1:C:763:LEU:HD11	1.68	0.75
1:F:679:ALA:O	1:F:791:ARG:NH2	2.21	0.74
1:B:1008:GLU:OE2	2:N:7:DC:N4	2.22	0.73

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	520/563 (92%)	498 (96%)	20 (4%)	2 (0%)	34	69
1	B	509/563 (90%)	488 (96%)	19 (4%)	2 (0%)	34	69
1	C	510/563 (91%)	490 (96%)	19 (4%)	1 (0%)	47	79
1	D	507/563 (90%)	488 (96%)	17 (3%)	2 (0%)	34	69
1	E	510/563 (91%)	492 (96%)	17 (3%)	1 (0%)	47	79

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	F	513/563 (91%)	488 (95%)	20 (4%)	5 (1%)	15	48
All	All	3069/3378 (91%)	2944 (96%)	112 (4%)	13 (0%)	34	69

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	759	ILE
1	B	759	ILE
1	D	759	ILE
1	F	807	PHE
1	F	1280	SER

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	
1	A	421/499 (84%)	411 (98%)	10 (2%)	49	77
1	B	398/499 (80%)	387 (97%)	11 (3%)	43	74
1	C	402/499 (81%)	392 (98%)	10 (2%)	47	76
1	D	374/499 (75%)	367 (98%)	7 (2%)	57	81
1	E	381/499 (76%)	366 (96%)	15 (4%)	32	65
1	F	360/499 (72%)	350 (97%)	10 (3%)	43	74
All	All	2336/2994 (78%)	2273 (97%)	63 (3%)	44	74

5 of 63 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	830	THR
1	D	942	VAL
1	F	922	LEU
1	C	843	THR
1	D	735	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 35 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	802	GLN
1	D	671	ASN
1	F	1019	HIS
1	C	996	HIS
1	C	1021	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 31 ligands modelled in this entry, 12 are monoatomic - leaving 19 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	RY8	C	1303	-	27,29,29	0.30	0	38,43,43	0.50	1 (2%)
5	RY8	D	1303	-	27,29,29	0.31	0	38,43,43	0.50	1 (2%)
5	RY8	A	1303	-	27,29,29	0.32	0	38,43,43	0.54	1 (2%)
5	RY8	B	1303	-	27,29,29	0.31	0	38,43,43	0.50	1 (2%)
4	ADP	D	1302	-	24,29,29	0.95	1 (4%)	29,45,45	1.43	4 (13%)
4	ADP	B	1302	-	24,29,29	0.95	1 (4%)	29,45,45	1.37	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	PG4	B	1304	-	12,12,12	0.11	0	11,11,11	0.12	0
6	PG4	D	1304	-	12,12,12	0.13	0	11,11,11	0.10	0
6	PG4	C	1304	-	12,12,12	0.12	0	11,11,11	0.10	0
6	PG4	C	1305	-	12,12,12	0.11	0	11,11,11	0.12	0
4	ADP	F	1302	1	24,29,29	0.95	1 (4%)	29,45,45	1.39	4 (13%)
6	PG4	A	1304	-	12,12,12	0.12	0	11,11,11	0.11	0
6	PG4	E	1304	-	12,12,12	0.11	0	11,11,11	0.11	0
6	PG4	A	1305	-	12,12,12	0.12	0	11,11,11	0.11	0
4	ADP	E	1302	-	24,29,29	0.95	1 (4%)	29,45,45	1.44	4 (13%)
4	ADP	C	1302	-	24,29,29	0.95	1 (4%)	29,45,45	1.39	3 (10%)
4	ADP	A	1302	-	24,29,29	0.94	1 (4%)	29,45,45	1.43	4 (13%)
5	RY8	E	1303	-	27,29,29	0.29	0	38,43,43	0.49	1 (2%)
5	RY8	F	1303	1	27,29,29	0.30	0	38,43,43	0.49	1 (2%)

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
5	RY8	C	1303	-	-	2/18/18/18	0/3/3/3
5	RY8	D	1303	-	-	2/18/18/18	0/3/3/3
5	RY8	A	1303	-	-	2/18/18/18	0/3/3/3
5	RY8	B	1303	-	-	6/18/18/18	0/3/3/3
4	ADP	D	1302	-	-	5/12/32/32	0/3/3/3
4	ADP	B	1302	-	-	5/12/32/32	0/3/3/3
6	PG4	B	1304	-	-	4/10/10/10	-
6	PG4	D	1304	-	-	4/10/10/10	-
6	PG4	C	1304	-	-	5/10/10/10	-
6	PG4	C	1305	-	-	3/10/10/10	-
4	ADP	F	1302	1	-	1/12/32/32	0/3/3/3
6	PG4	A	1304	-	-	2/10/10/10	-
6	PG4	E	1304	-	-	5/10/10/10	-
6	PG4	A	1305	-	-	7/10/10/10	-
4	ADP	E	1302	-	-	1/12/32/32	0/3/3/3
4	ADP	C	1302	-	-	3/12/32/32	0/3/3/3
4	ADP	A	1302	-	-	5/12/32/32	0/3/3/3
5	RY8	E	1303	-	-	2/18/18/18	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	RY8	F	1303	1	-	5/18/18/18	0/3/3/3

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	E	1302	ADP	C5-C4	2.49	1.47	1.40
4	D	1302	ADP	C5-C4	2.48	1.47	1.40
4	A	1302	ADP	C5-C4	2.47	1.47	1.40
4	C	1302	ADP	C5-C4	2.47	1.47	1.40
4	F	1302	ADP	C5-C4	2.46	1.47	1.40

The worst 5 of 29 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	E	1302	ADP	PA-O3A-PB	-3.52	120.75	132.83
4	A	1302	ADP	PA-O3A-PB	-3.44	121.01	132.83
4	D	1302	ADP	PA-O3A-PB	-3.36	121.29	132.83
4	F	1302	ADP	N3-C2-N1	-3.27	123.57	128.68
4	A	1302	ADP	N3-C2-N1	-3.25	123.59	128.68

There are no chirality outliers.

5 of 69 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1302	ADP	PA-O3A-PB-O2B
4	D	1302	ADP	C5'-O5'-PA-O1A
4	C	1302	ADP	PA-O3A-PB-O2B
4	B	1302	ADP	PA-O3A-PB-O2B
4	B	1302	ADP	PA-O3A-PB-O3B

There are no ring outliers.

10 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	1303	RY8	1	0
6	B	1304	PG4	1	0
6	D	1304	PG4	1	0
6	C	1304	PG4	1	0
6	C	1305	PG4	1	0
4	F	1302	ADP	1	0
6	A	1304	PG4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1305	PG4	1	0
4	C	1302	ADP	1	0
5	E	1303	RY8	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 RY8 C 1303

Bond lengths   Bond angles
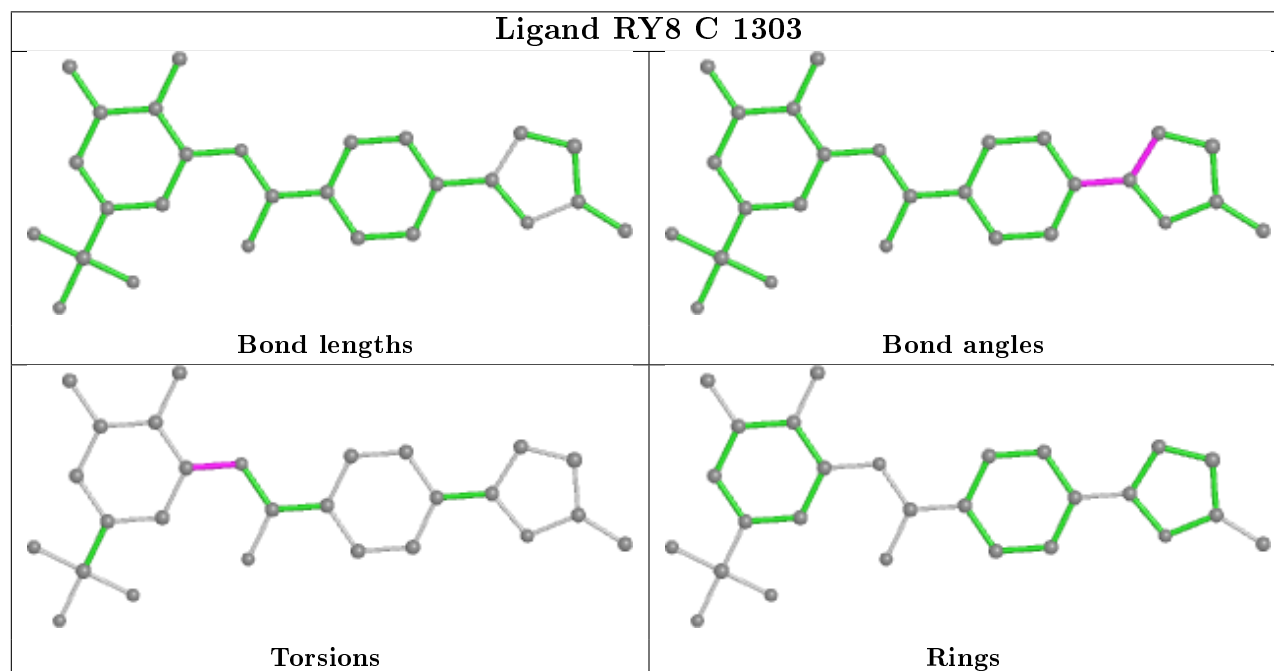
Torsions   Rings
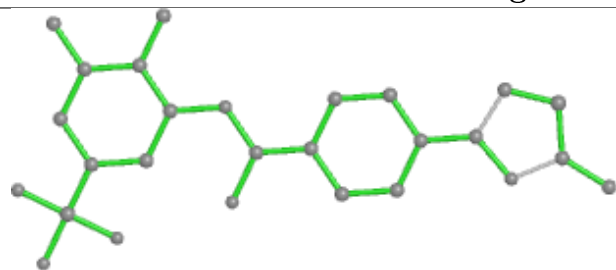
Ligand RY8 D 1303

Bond lengths
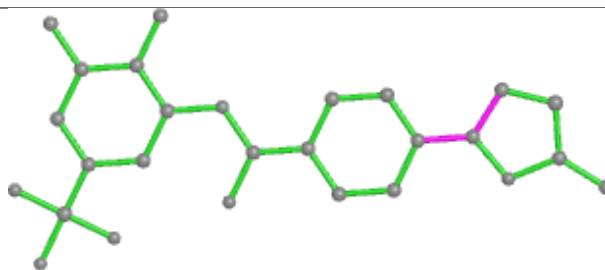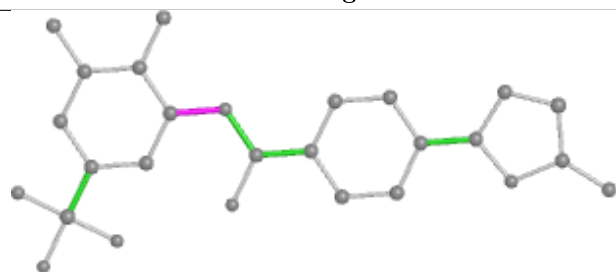
Bond angles
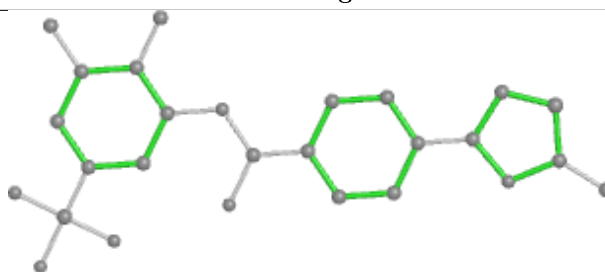
Torsions

Rings

Ligand RY8 A 1303
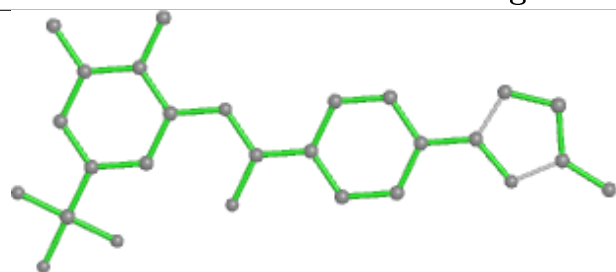
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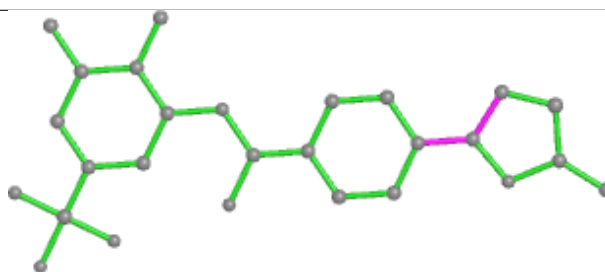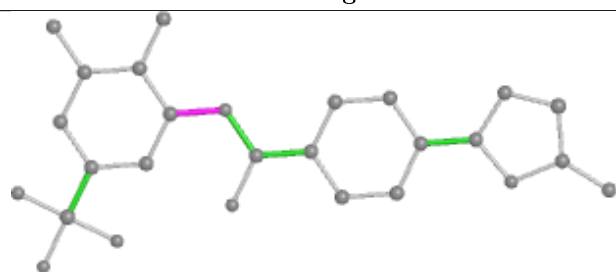
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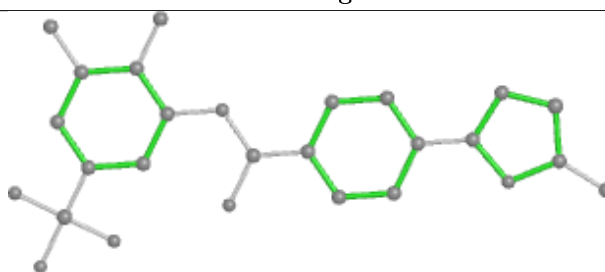
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Rings

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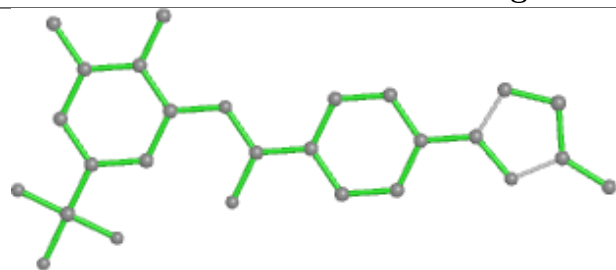
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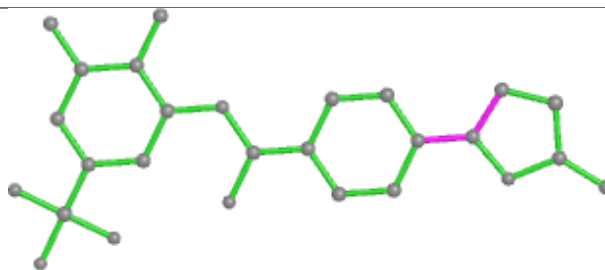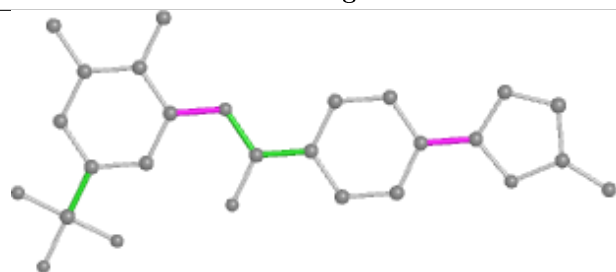
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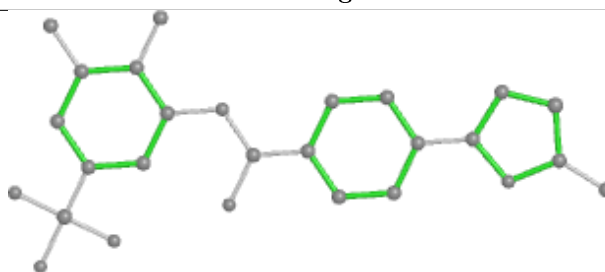
Torsions

Rings

Ligand ADP D 1302
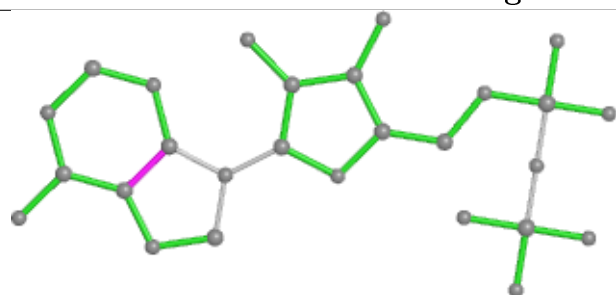
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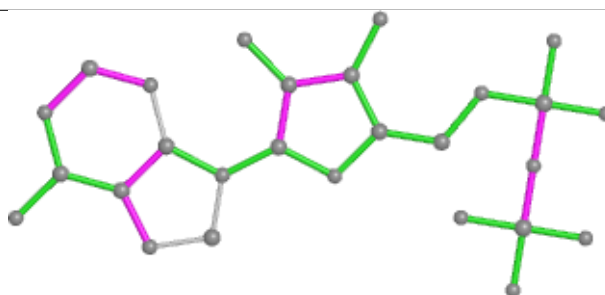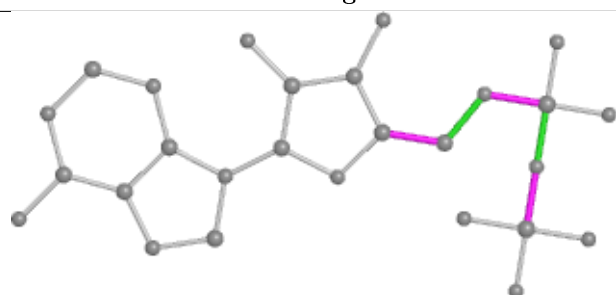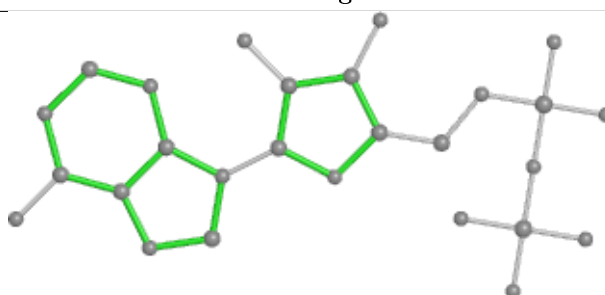
Bond angles

Torsions

Rings

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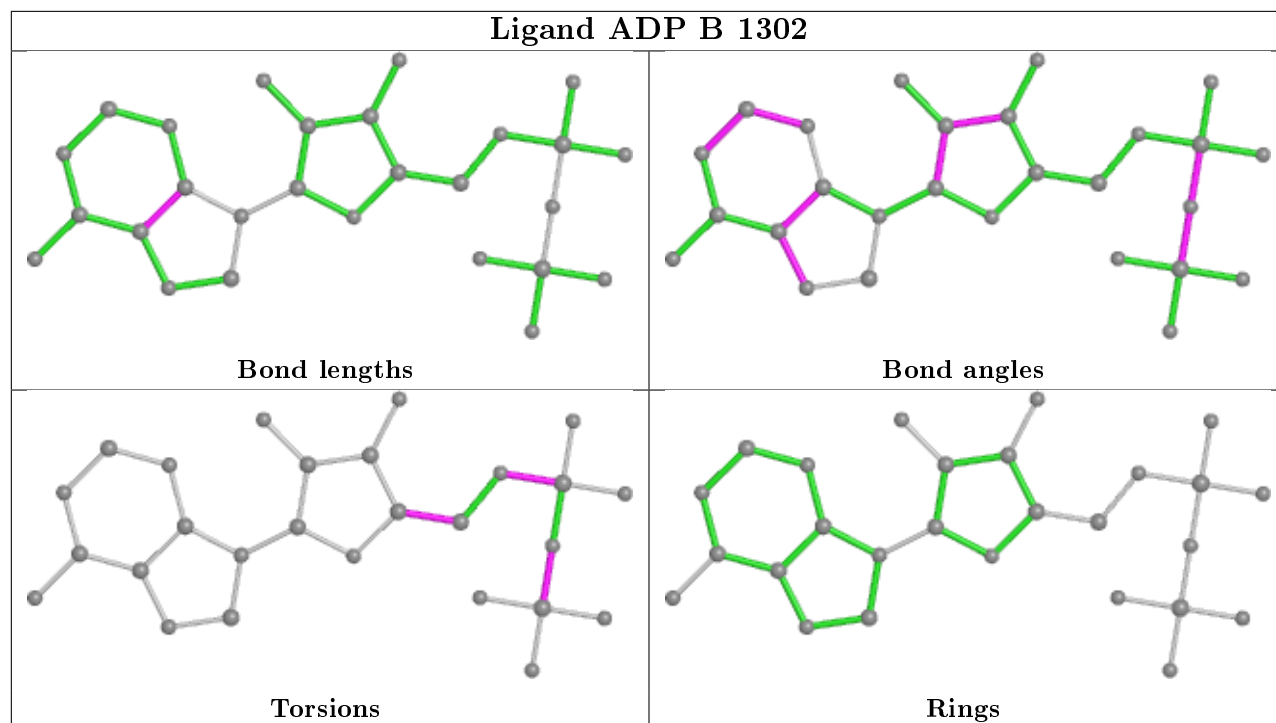
Bond lengths

Bond angles

Torsions

Rings

Ligand ADP F 1302

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP E 1302

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP C 1302

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 1302

Bond lengths

Bond angles

Torsions

Rings

Ligand RY8 E 1303

Bond lengths

Bond angles

Torsions

Rings

Ligand RY8 F 1303

Bond lengths

Bond angles

Torsions

Rings
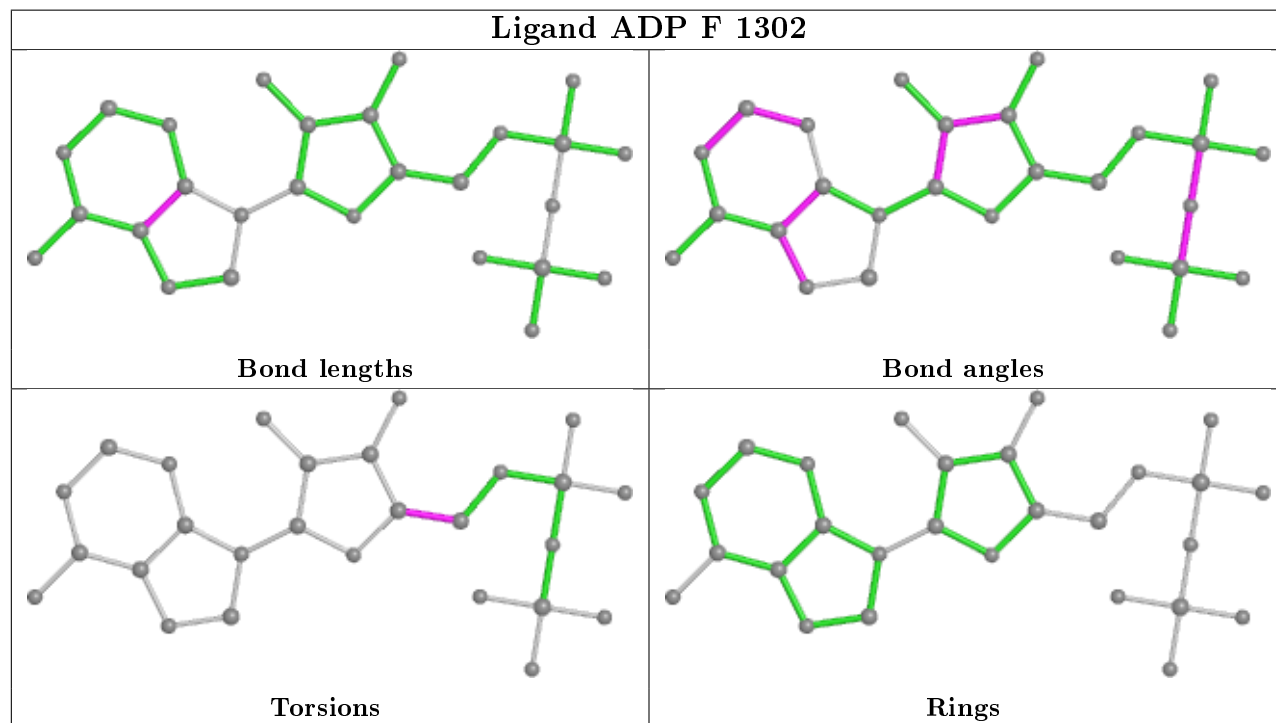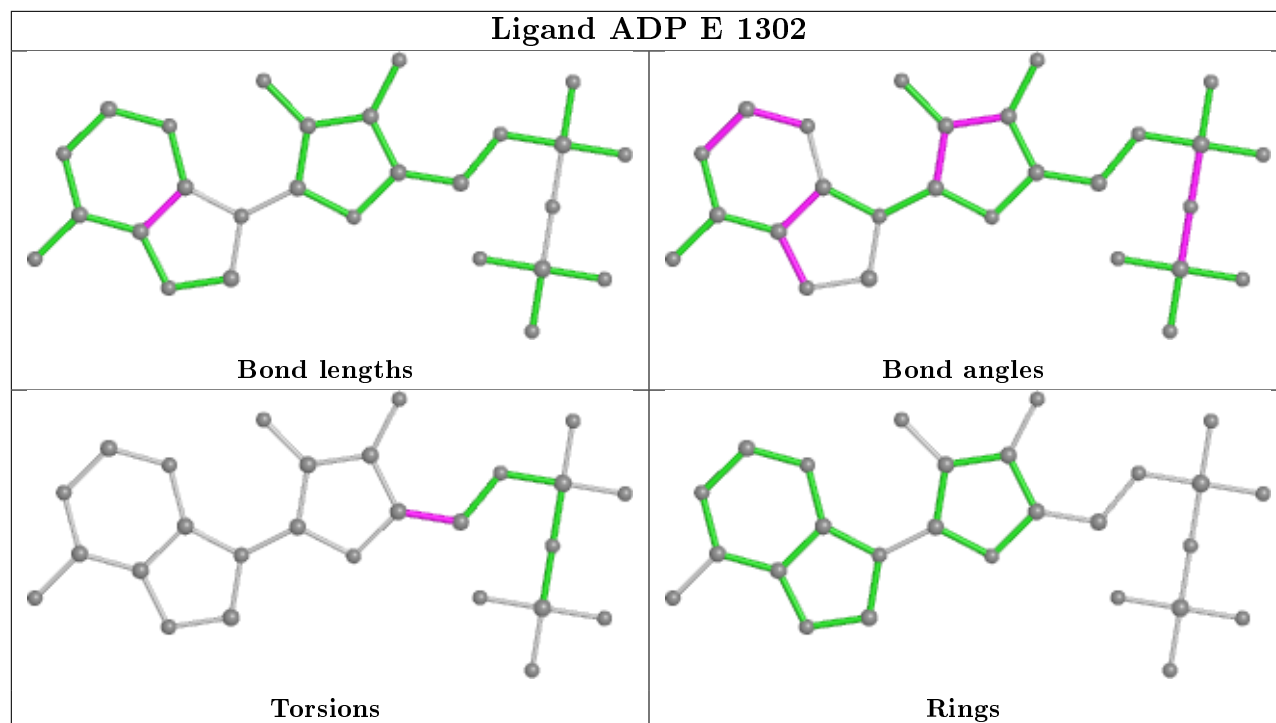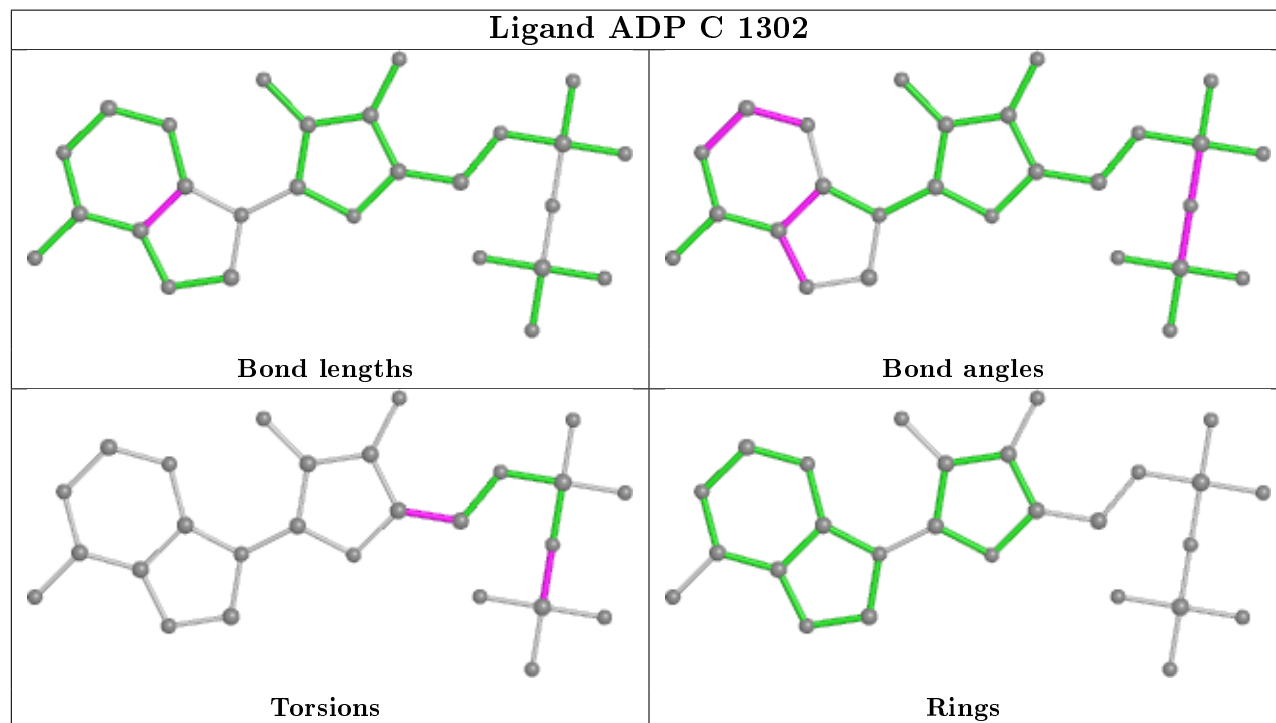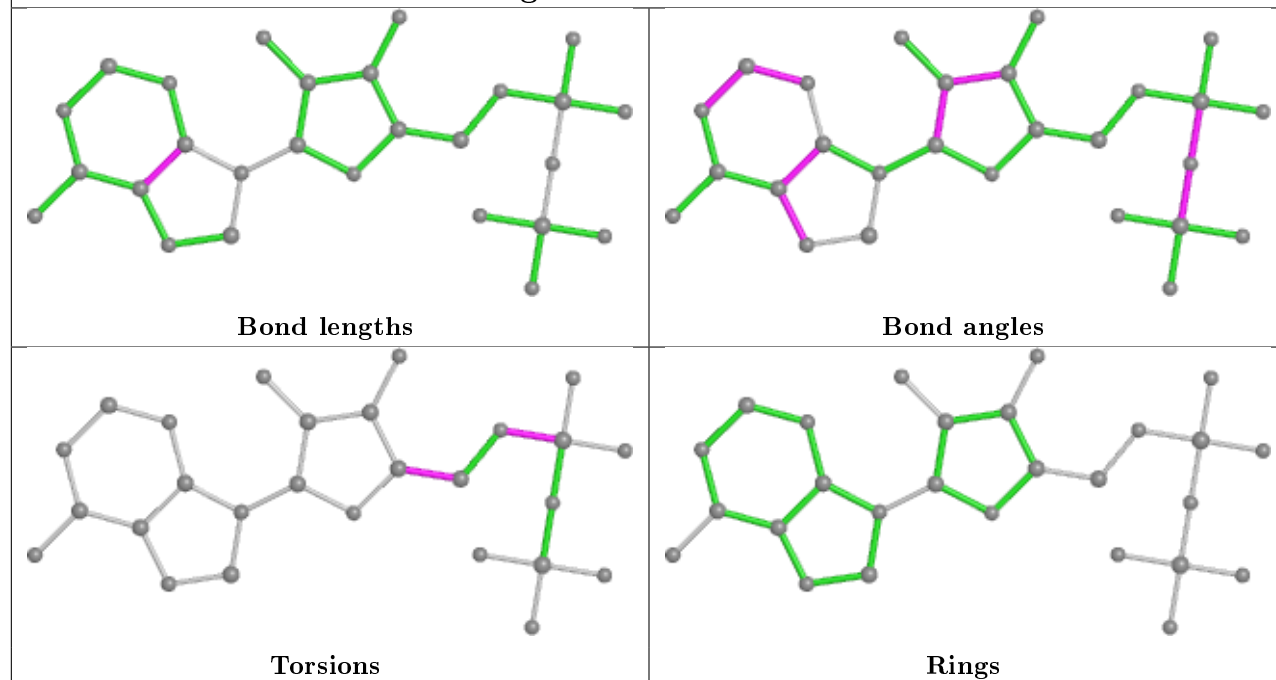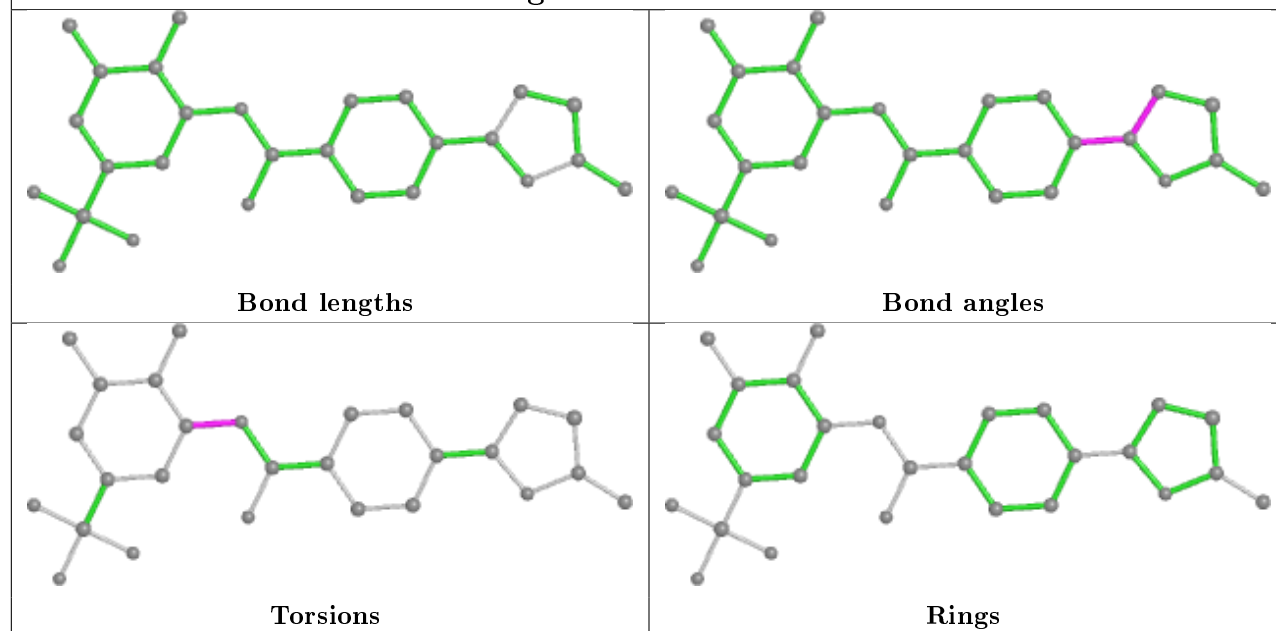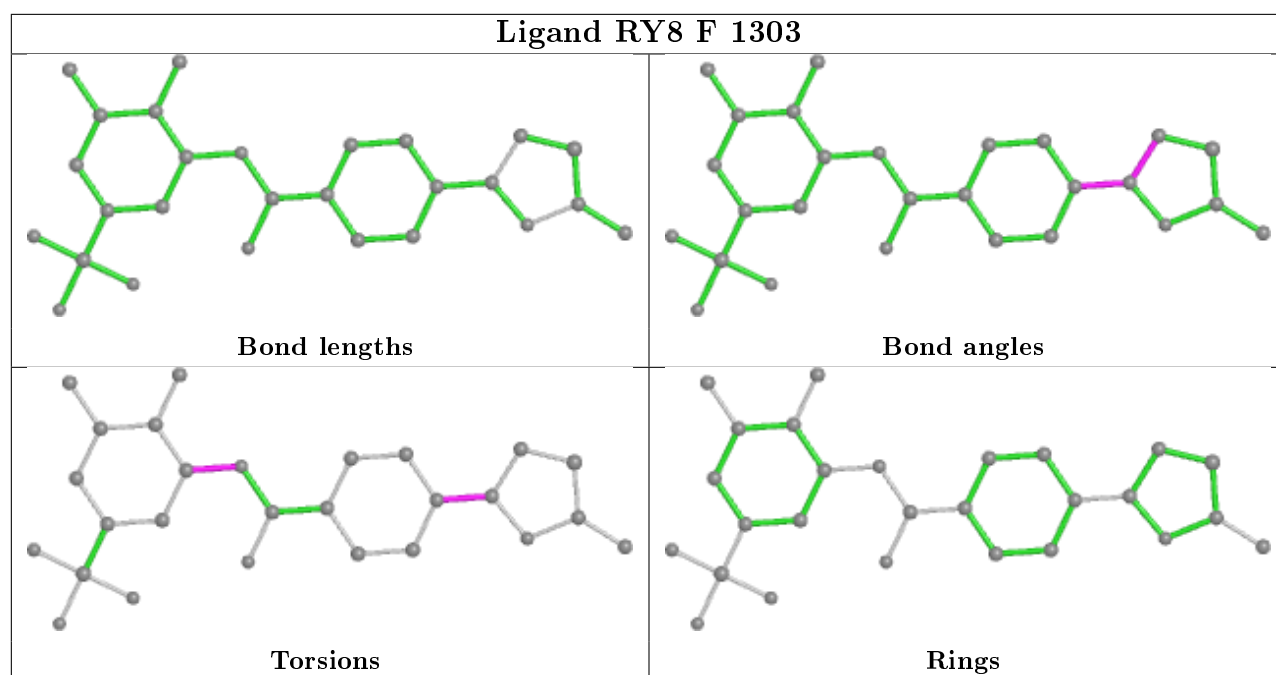
5.7 Other polymers (i)

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	A	522/563 (92%)	0.35	19 (3%)	42	28	49, 71, 125, 194	1 (0%)
1	B	513/563 (91%)	0.27	12 (2%)	60	43	51, 79, 143, 197	1 (0%)
1	C	513/563 (91%)	0.29	13 (2%)	57	40	53, 84, 143, 194	1 (0%)
1	D	510/563 (90%)	0.32	23 (4%)	33	21	53, 94, 156, 213	2 (0%)
1	E	513/563 (91%)	0.37	24 (4%)	31	20	57, 94, 147, 193	2 (0%)
1	F	516/563 (91%)	0.53	47 (9%)	9	5	66, 101, 153, 229	2 (0%)
2	M	13/15 (86%)	0.11	0	100	100	63, 84, 121, 129	0
2	N	13/15 (86%)	-0.19	0	100	100	61, 80, 143, 150	0
2	O	13/15 (86%)	-0.08	0	100	100	70, 101, 145, 158	0
2	P	13/15 (86%)	-0.17	0	100	100	68, 93, 124, 153	0
2	Q	13/15 (86%)	-0.01	0	100	100	78, 100, 137, 164	0
2	R	13/15 (86%)	-0.32	0	100	100	105, 121, 157, 163	0
All	All	3165/3468 (91%)	0.34	138 (4%)	34	21	49, 88, 146, 229	9 (0%)

The worst 5 of 138 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	905	ALA	5.2
1	D	1256	ASP	5.2
1	F	989	CYS	4.9
1	F	901	CYS	4.8
1	D	990	LEU	4.7

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
7	MG	F	1304	1/1	0.42	0.33	94,94,94,94	0
7	MG	N	101	1/1	0.52	0.30	69,69,69,69	0
6	PG4	C	1305	13/13	0.74	0.37	83,98,103,104	0
6	PG4	A	1305	13/13	0.77	0.36	84,93,99,102	0
6	PG4	C	1304	13/13	0.81	0.27	85,92,100,101	0
7	MG	P	101	1/1	0.81	0.11	67,67,67,67	0
6	PG4	E	1304	13/13	0.85	0.22	83,90,93,97	0
6	PG4	B	1304	13/13	0.86	0.35	79,84,94,95	0
6	PG4	D	1304	13/13	0.87	0.38	86,92,100,101	0
4	ADP	F	1302	27/27	0.88	0.29	70,86,96,110	0
7	MG	Q	101	1/1	0.89	0.16	79,79,79,79	0
7	MG	Q	102	1/1	0.89	0.35	77,77,77,77	0
4	ADP	E	1302	27/27	0.90	0.19	88,100,111,113	0
4	ADP	D	1302	27/27	0.90	0.23	76,99,108,113	0
6	PG4	A	1304	13/13	0.91	0.33	74,77,84,89	0
7	MG	M	100	1/1	0.91	0.35	69,69,69,69	0
5	RY8	F	1303	27/27	0.91	0.29	78,83,89,94	0
4	ADP	C	1302	27/27	0.92	0.20	58,73,82,85	0
5	RY8	D	1303	27/27	0.93	0.24	68,85,99,108	0
4	ADP	B	1302	27/27	0.94	0.16	62,74,80,82	0
4	ADP	A	1302	27/27	0.94	0.18	61,69,81,83	0
5	RY8	C	1303	27/27	0.94	0.32	57,71,80,96	0
3	ZN	C	1301	1/1	0.95	0.20	95,95,95,95	0
5	RY8	E	1303	27/27	0.95	0.31	63,76,79,88	0
5	RY8	B	1303	27/27	0.96	0.26	45,59,66,82	0
3	ZN	A	1301	1/1	0.96	0.22	70,70,70,70	0
3	ZN	D	1301	1/1	0.96	0.16	113,113,113,113	0
5	RY8	A	1303	27/27	0.96	0.22	43,51,61,82	0
3	ZN	E	1301	1/1	0.97	0.17	121,121,121,121	0
3	ZN	F	1301	1/1	0.98	0.13	103,103,103,103	0
3	ZN	B	1301	1/1	0.98	0.20	94,94,94,94	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 F 1302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
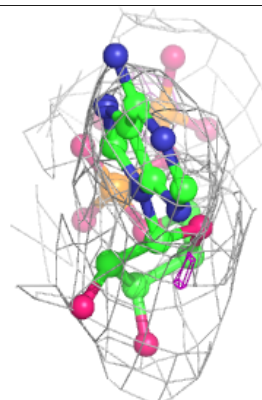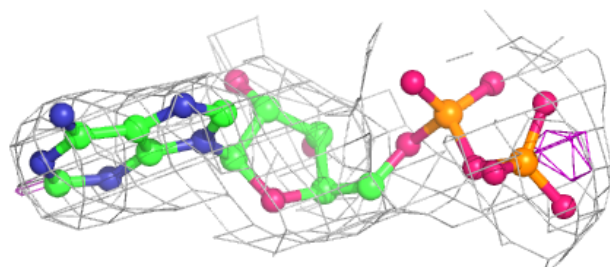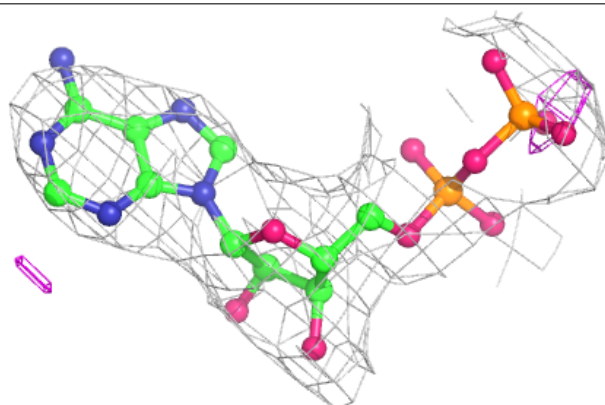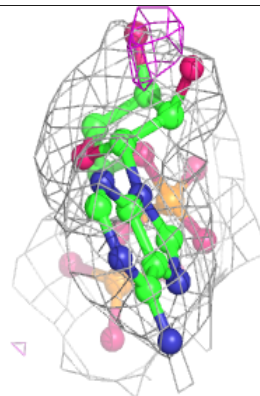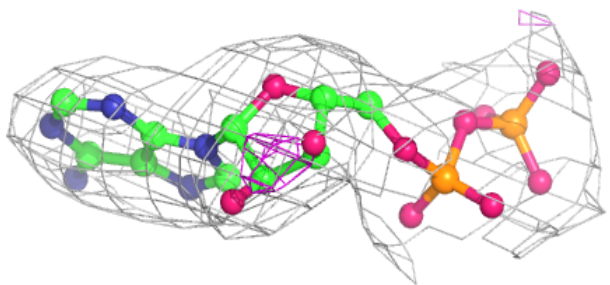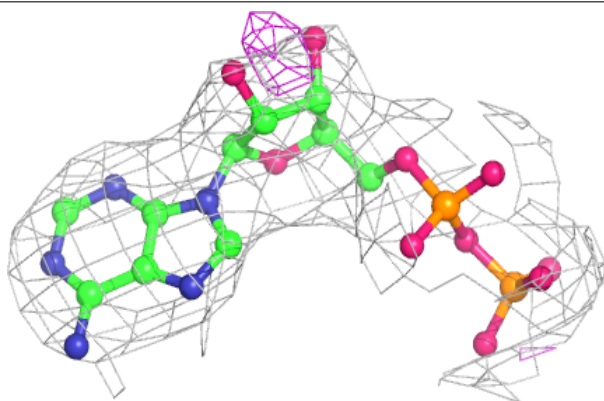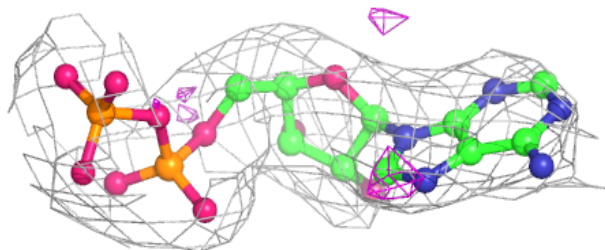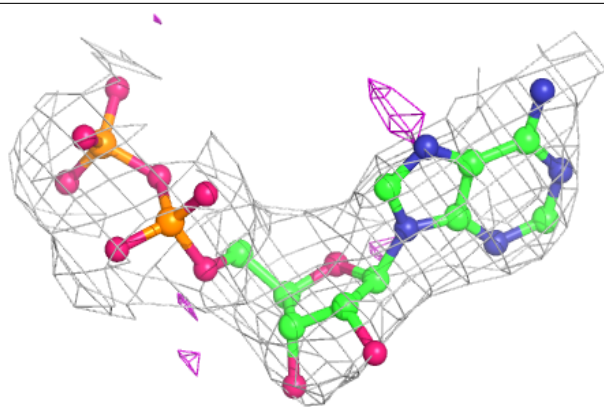mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
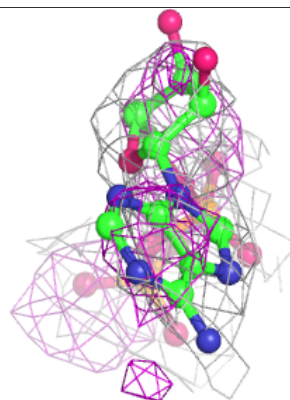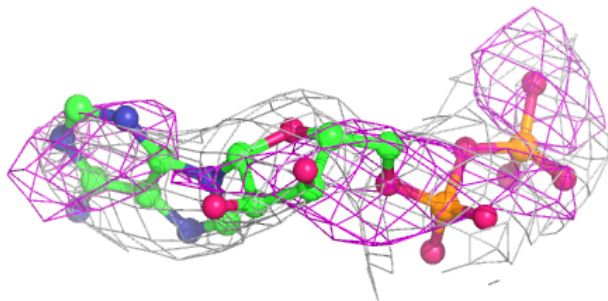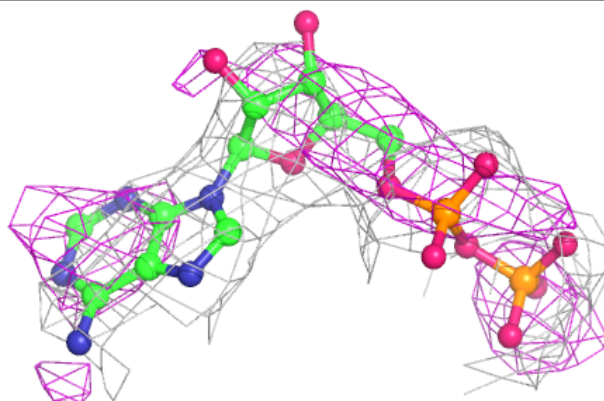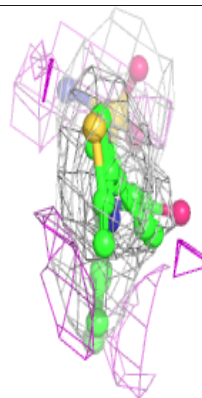
Electron density around ADP E 1302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
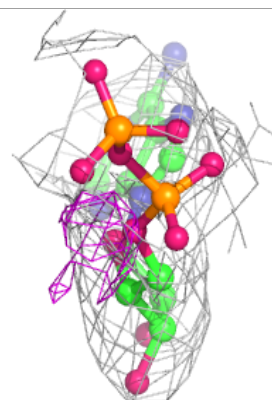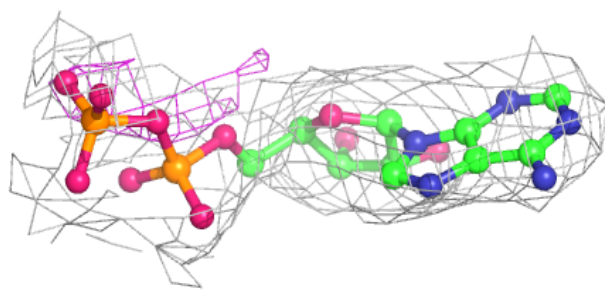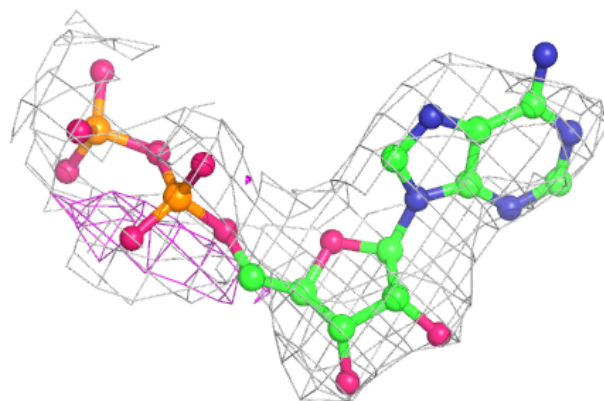
Electron density around ADP D 1302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
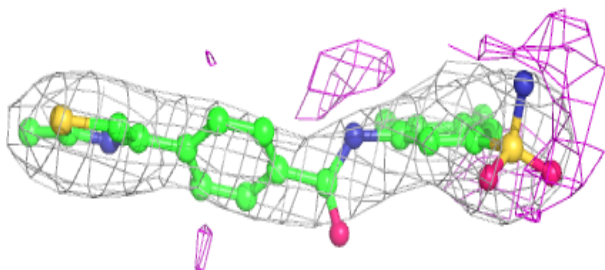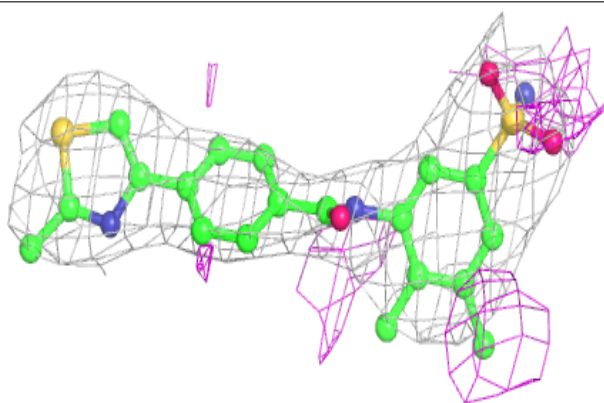mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
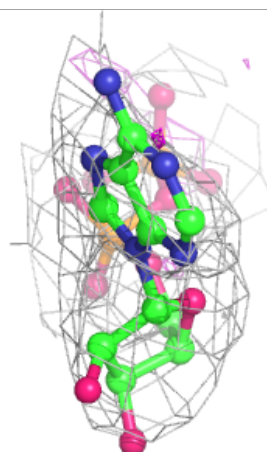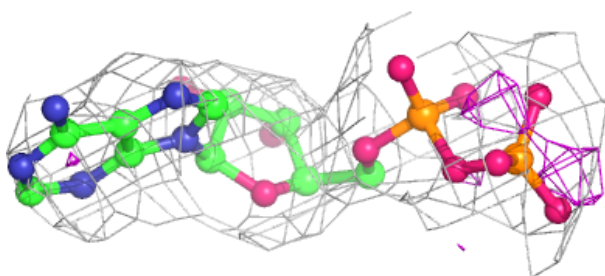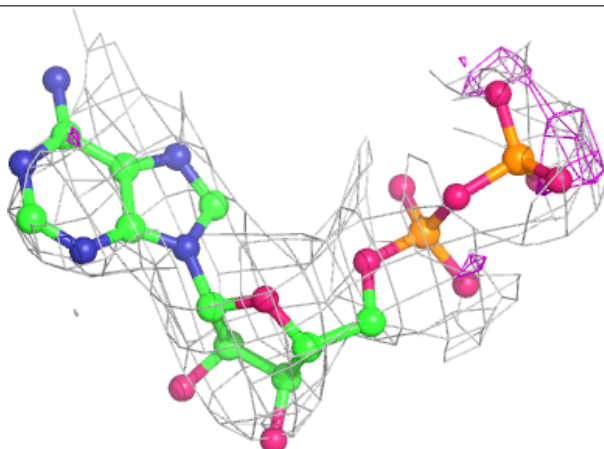
Electron density around RY8 F 1303:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
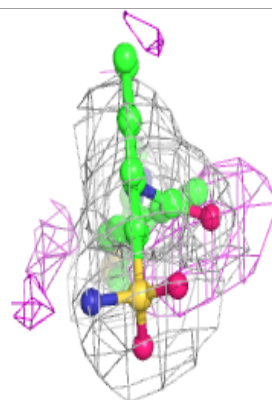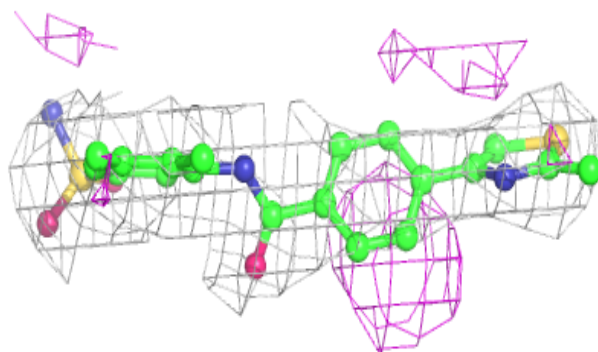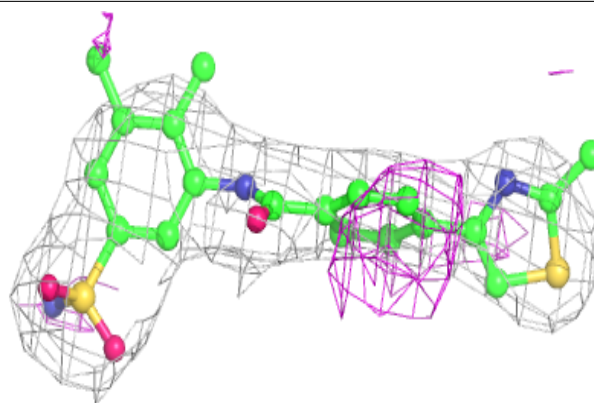
Electron density around ADP C 1302:

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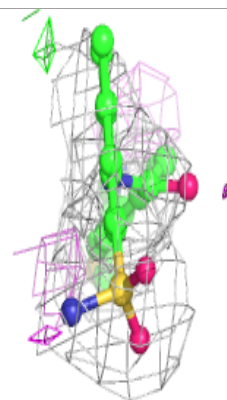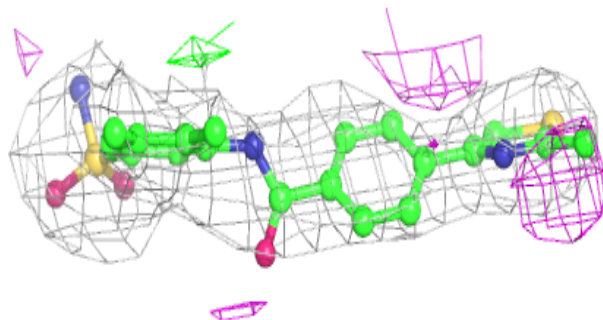$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
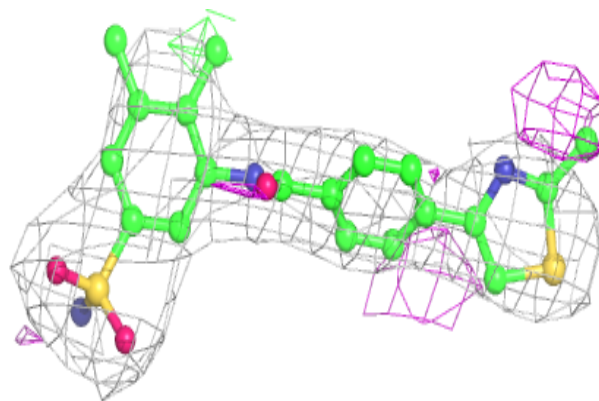and green (positive)

Electron density around RY8 D 1303:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
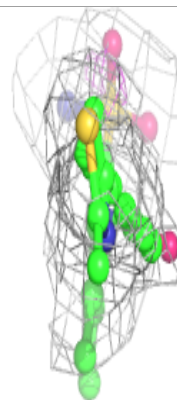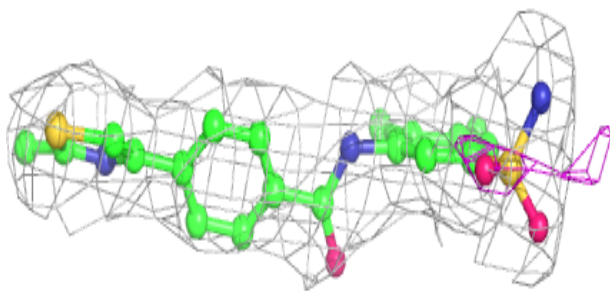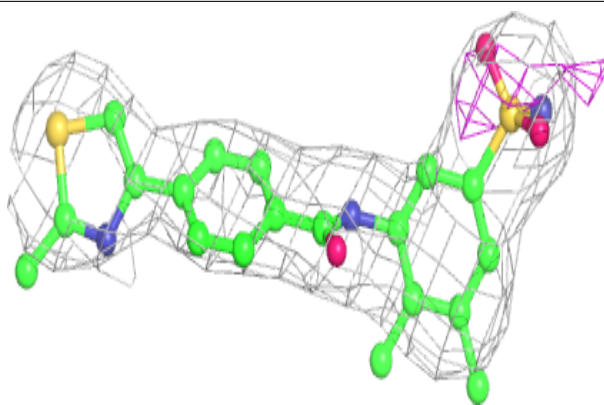
Electron density around ADP B 1302:

$2mF_o$-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 1302:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
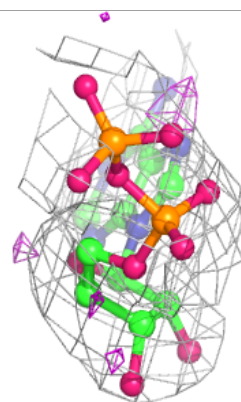
Electron density around RY8 C 1303:

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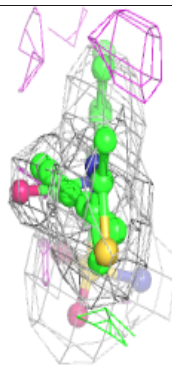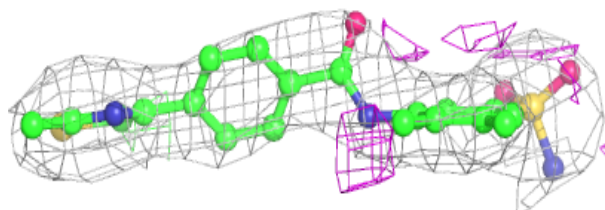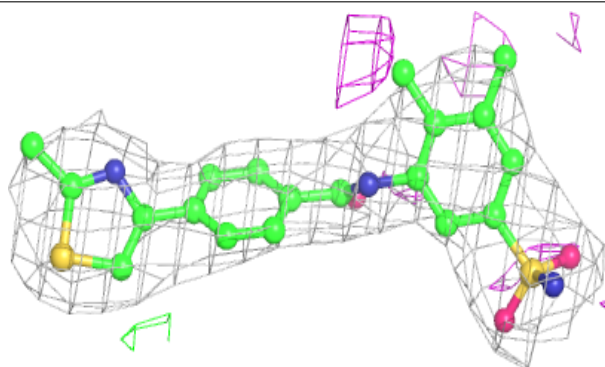and green (positive)

Electron density around RY8 E 1303:

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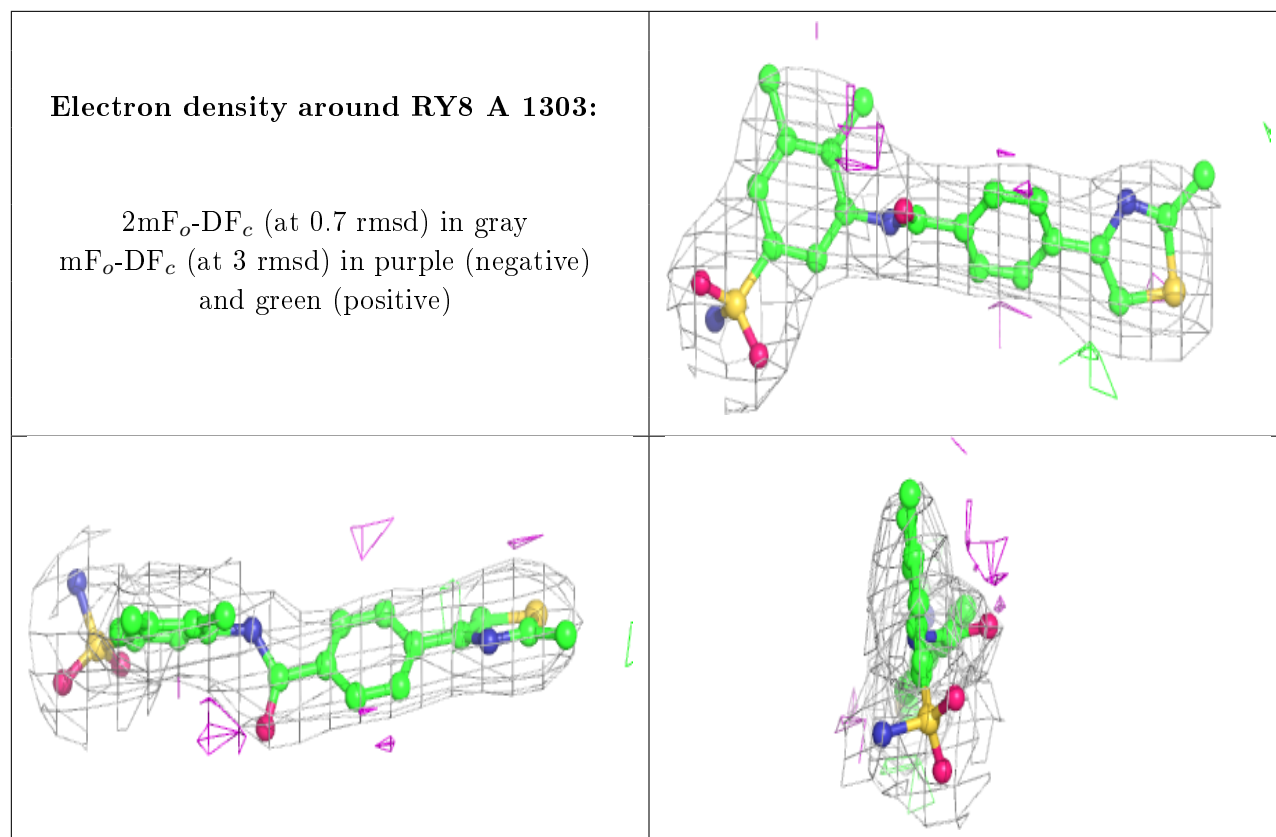mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around RY8 B 1303:

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

Electron density around RY8 A 1303:

$2mF_o$-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.