



# wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 25, 2020 – 05:58 PM BST

PDB ID : 5OCH  
Title : The crystal structure of human ABCB8 in an outward-facing state  
Authors : Faust, B.; Pike, A.C.W.; Shintre, C.A.; Quigley, A.M.; Chu, A.; Barr, A.; Shrestha, L.; Mukhopadhyay, S.; Borkowska, O.; Chalk, R.; Burgess-Brown, N.A.; Arrowsmith, C.H.; Edwards, A.M.; Bountra, C.; Carpenter, E.P.; Structural Genomics Consortium (SGC)  
Deposited on : 2017-06-30  
Resolution : 3.40 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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	:	2.13
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)	:	2.13

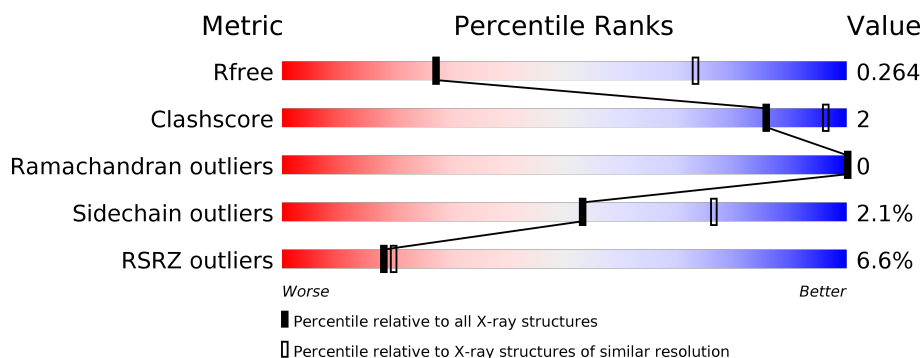
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	612	<div> <div>3%</div> <div>83% 7% 10%</div> </div>
1	C	612	<div> <div>10%</div> <div>84% 12%</div> </div>
1	D	612	<div> <div>5%</div> <div>88% 6% 6%</div> </div>
2	B	612	<div> <div>3%</div> <div>88% 6% 6%</div> </div>
3	E	612	<div> <div>12%</div> <div>89% 5% 6%</div> </div>
4	F	612	<div> <div>3%</div> <div>85% 8% 6%</div> </div>

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Mol	Chain	Length	Quality of chain
4	G	612	<div><div></div><div>3%</div><div>85%</div><div>5%</div><div>10%</div></div>
5	H	612	<div><div></div><div>9%</div><div>84%</div><div>5%</div><div>10%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 31278 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 ATP-binding cassette sub-family B member 8, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	552	Total	C	N	O	S	0	0	0
			3910	2479	676	733	22			
1	C	537	Total	C	N	O	S	0	0	0
			3541	2229	626	670	16			
1	D	573	Total	C	N	O	S	0	0	0
			3937	2502	682	731	22			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	110	MET	-	initiating methionine	UNP Q9NUT2
A	715	ALA	-	expression tag	UNP Q9NUT2
A	716	GLU	-	expression tag	UNP Q9NUT2
A	717	ASN	-	expression tag	UNP Q9NUT2
A	718	LEU	-	expression tag	UNP Q9NUT2
A	719	TYR	-	expression tag	UNP Q9NUT2
A	720	PHE	-	expression tag	UNP Q9NUT2
A	721	GLN	-	expression tag	UNP Q9NUT2
C	110	MET	-	initiating methionine	UNP Q9NUT2
C	715	ALA	-	expression tag	UNP Q9NUT2
C	716	GLU	-	expression tag	UNP Q9NUT2
C	717	ASN	-	expression tag	UNP Q9NUT2
C	718	LEU	-	expression tag	UNP Q9NUT2
C	719	TYR	-	expression tag	UNP Q9NUT2
C	720	PHE	-	expression tag	UNP Q9NUT2
C	721	GLN	-	expression tag	UNP Q9NUT2
D	110	MET	-	initiating methionine	UNP Q9NUT2
D	715	ALA	-	expression tag	UNP Q9NUT2
D	716	GLU	-	expression tag	UNP Q9NUT2
D	717	ASN	-	expression tag	UNP Q9NUT2
D	718	LEU	-	expression tag	UNP Q9NUT2
D	719	TYR	-	expression tag	UNP Q9NUT2
D	720	PHE	-	expression tag	UNP Q9NUT2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	721	GLN	-	expression tag	UNP Q9NUT2

- Molecule 2 is a protein called ATP-binding cassette sub-family B member 8, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	573	Total	C	N	O	S	0	0	0
			4051	2562	715	753	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	110	MET	-	initiating methionine	UNP Q9NUT2
B	715	ALA	-	expression tag	UNP Q9NUT2
B	716	GLU	-	expression tag	UNP Q9NUT2
B	717	ASN	-	expression tag	UNP Q9NUT2
B	718	LEU	-	expression tag	UNP Q9NUT2
B	719	TYR	-	expression tag	UNP Q9NUT2
B	720	PHE	-	expression tag	UNP Q9NUT2
B	721	GLN	-	expression tag	UNP Q9NUT2

- Molecule 3 is a protein called ATP-binding cassette sub-family B member 8, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	576	Total	C	N	O	S	0	0	0
			3947	2495	697	734	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	110	MET	-	initiating methionine	UNP Q9NUT2
E	715	ALA	-	expression tag	UNP Q9NUT2
E	716	GLU	-	expression tag	UNP Q9NUT2
E	717	ASN	-	expression tag	UNP Q9NUT2
E	718	LEU	-	expression tag	UNP Q9NUT2
E	719	TYR	-	expression tag	UNP Q9NUT2
E	720	PHE	-	expression tag	UNP Q9NUT2
E	721	GLN	-	expression tag	UNP Q9NUT2

- Molecule 4 is a protein called ATP-binding cassette sub-family B member 8, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	573	Total	C	N	O	S	0	0	0
			4047	2567	700	756	24			
4	G	552	Total	C	N	O	S	0	0	0
			3812	2409	663	720	20			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	110	MET	-	initiating methionine	UNP Q9NUT2
F	715	ALA	-	expression tag	UNP Q9NUT2
F	716	GLU	-	expression tag	UNP Q9NUT2
F	717	ASN	-	expression tag	UNP Q9NUT2
F	718	LEU	-	expression tag	UNP Q9NUT2
F	719	TYR	-	expression tag	UNP Q9NUT2
F	720	PHE	-	expression tag	UNP Q9NUT2
F	721	GLN	-	expression tag	UNP Q9NUT2
G	110	MET	-	initiating methionine	UNP Q9NUT2
G	715	ALA	-	expression tag	UNP Q9NUT2
G	716	GLU	-	expression tag	UNP Q9NUT2
G	717	ASN	-	expression tag	UNP Q9NUT2
G	718	LEU	-	expression tag	UNP Q9NUT2
G	719	TYR	-	expression tag	UNP Q9NUT2
G	720	PHE	-	expression tag	UNP Q9NUT2
G	721	GLN	-	expression tag	UNP Q9NUT2

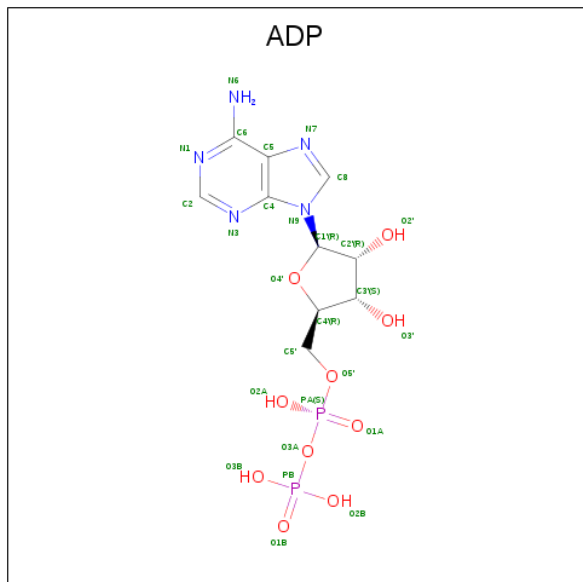
- Molecule 5 is a protein called ATP-binding cassette sub-family B member 8, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	H	548	Total	C	N	O	S	0	0	0
			3606	2255	639	691	21			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	110	MET	-	initiating methionine	UNP Q9NUT2
H	715	ALA	-	expression tag	UNP Q9NUT2
H	716	GLU	-	expression tag	UNP Q9NUT2
H	717	ASN	-	expression tag	UNP Q9NUT2
H	718	LEU	-	expression tag	UNP Q9NUT2
H	719	TYR	-	expression tag	UNP Q9NUT2
H	720	PHE	-	expression tag	UNP Q9NUT2
H	721	GLN	-	expression tag	UNP Q9NUT2

- 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
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	E	1	Total Mg 1 1	0	0
7	H	1	Total Mg 1 1	0	0
7	B	1	Total Mg 1 1	0	0
7	C	1	Total Mg 1 1	0	0
7	A	1	Total Mg 1 1	0	0
7	F	1	Total Mg 1 1	0	0

- Y01

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total 30	C 26	O 4	0	0
8	B	1	Total 35	C 31	O 4	0	0
8	D	1	Total 26	C 24	O 2	0	0
8	E	1	Total 28	C 24	O 4	0	0
8	F	1	Total 35	C 31	O 4	0	0





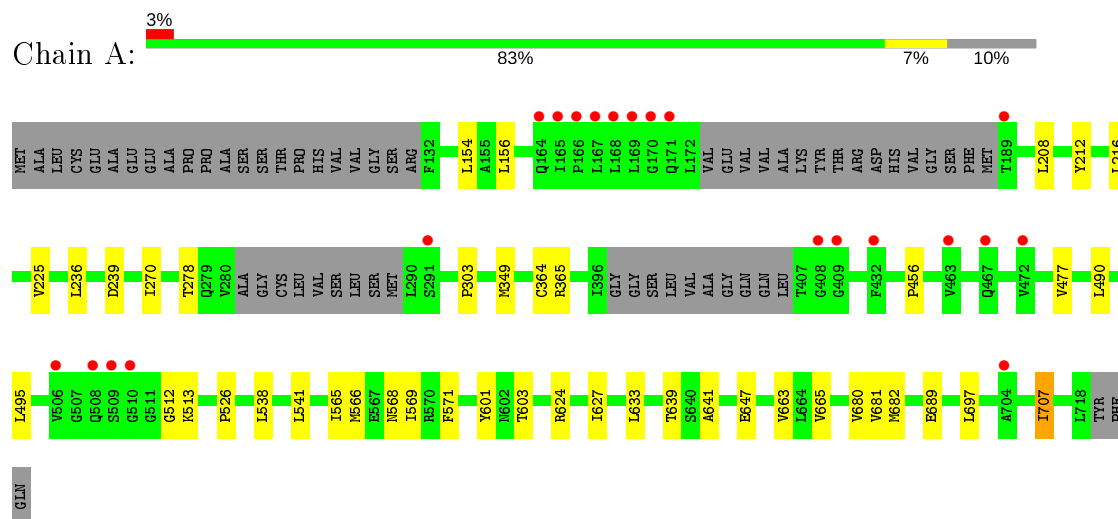
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	G	1	Total	C	O	0	0
			21	20	1		
8	H	1	Total	C	O	0	0
			28	24	4		

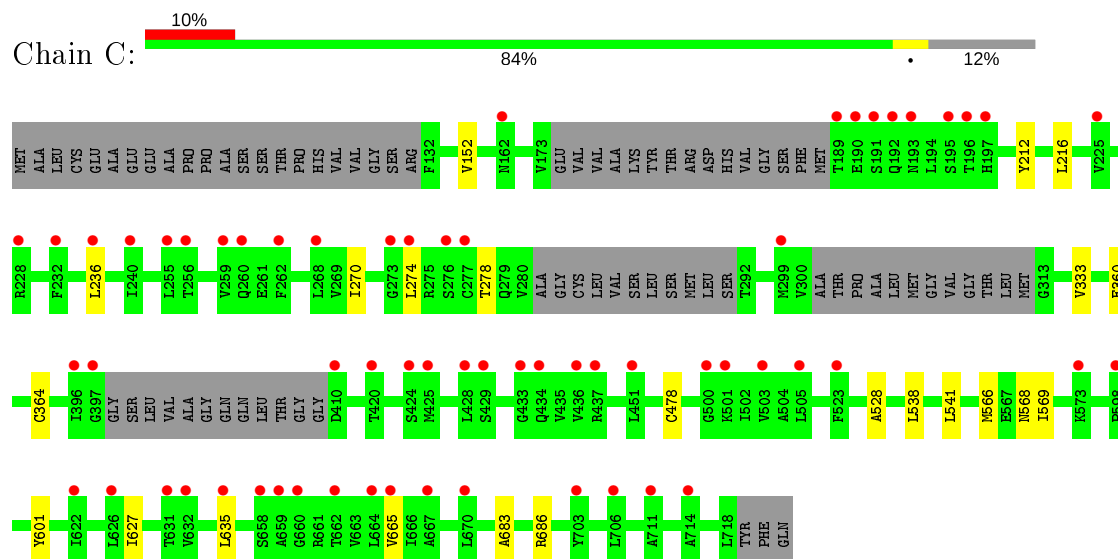
### 3 Residue-property plots [i](#)

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: ATP-binding cassette sub-family B member 8, mitochondrial

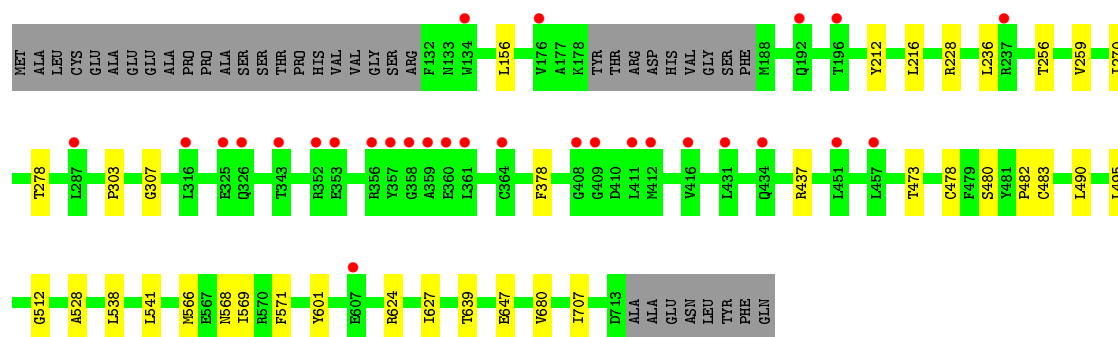


- Molecule 1: ATP-binding cassette sub-family B member 8, mitochondrial

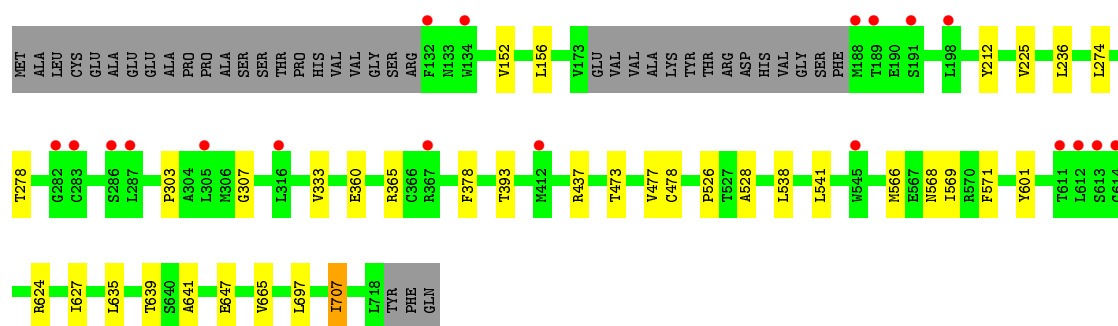
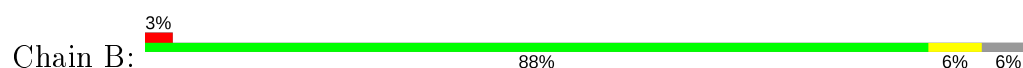


- Molecule 1: ATP-binding cassette sub-family B member 8, mitochondrial

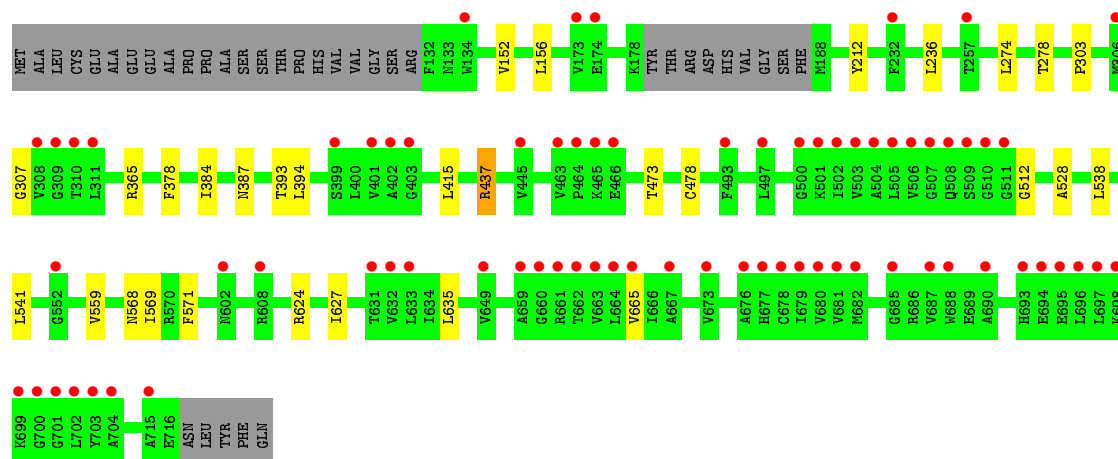
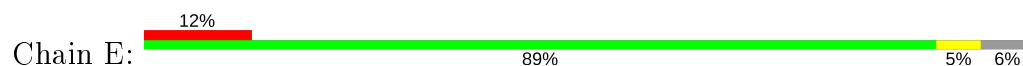




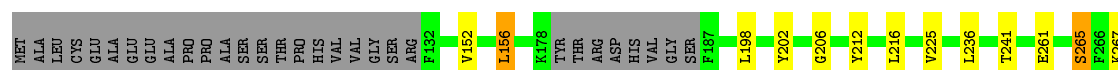
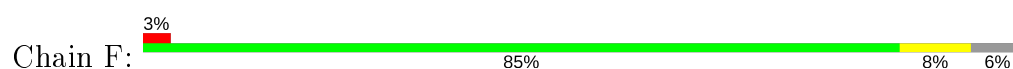
- Molecule 2: ATP-binding cassette sub-family B member 8, mitochondrial

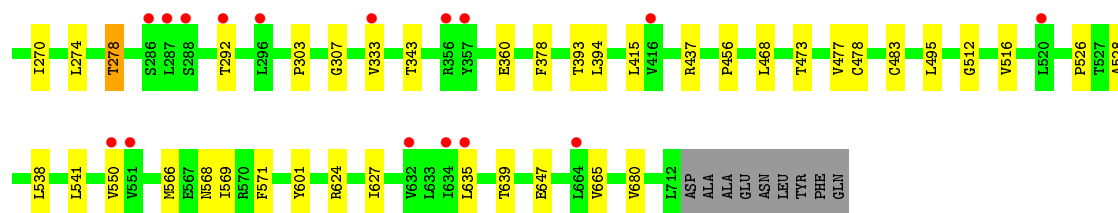


- Molecule 3: ATP-binding cassette sub-family B member 8, mitochondrial

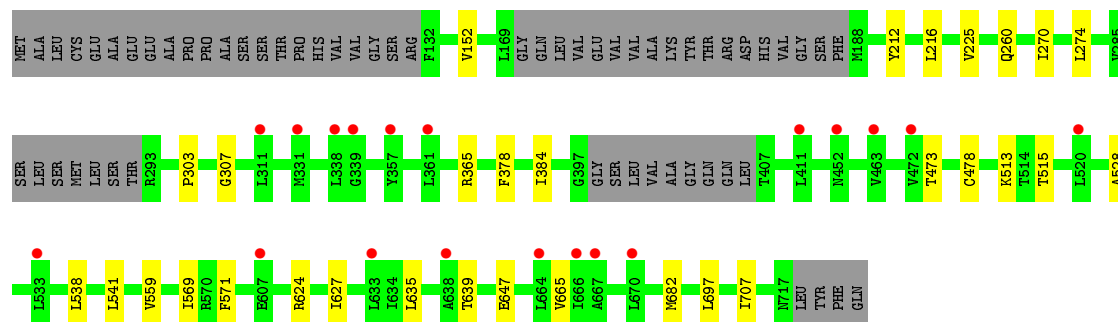
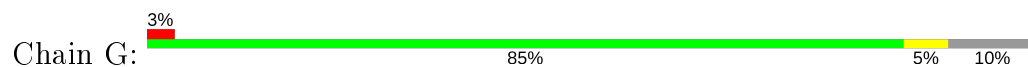


- Molecule 4: ATP-binding cassette sub-family B member 8, mitochondrial

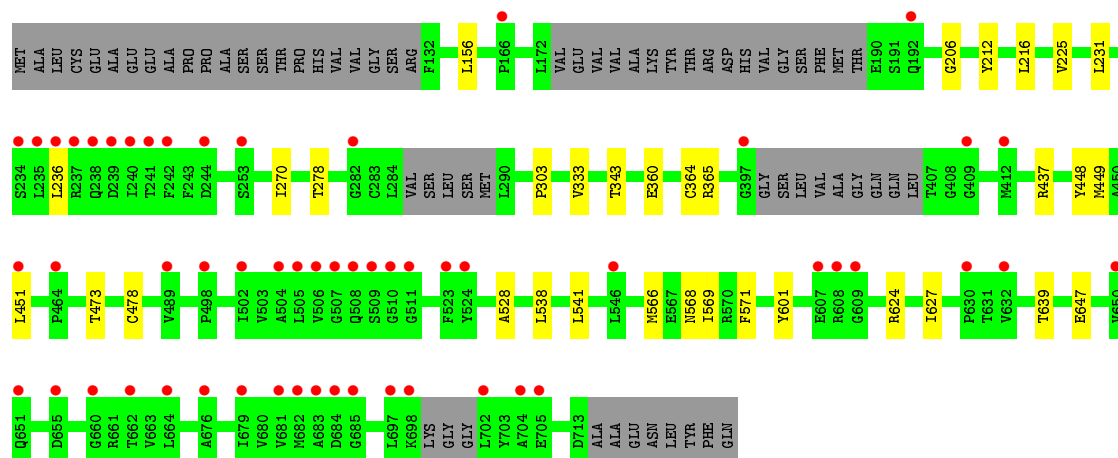
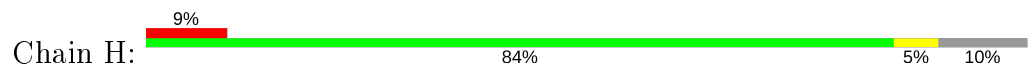




- Molecule 4: ATP-binding cassette sub-family B member 8, mitochondrial



- Molecule 5: ATP-binding cassette sub-family B member 8, mitochondrial



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	181.08Å 98.50Å 214.87Å 90.00° 90.50° 90.00°	Depositor
Resolution (Å)	72.61 – 3.40 72.60 – 3.40	Depositor EDS
% Data completeness (in resolution range)	61.9 (72.61-3.40) 60.6 (72.60-3.40)	Depositor EDS
$R_{merge}$	0.22	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.70 (at 3.41Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.231 , 0.251 0.249 , 0.264	Depositor DCC
$R_{free}$ test set	3147 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	107.9	Xtriage
Anisotropy	0.150	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.27 , 98.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.24$	Xtriage
Estimated twinning fraction	0.104 for h,-k,-l	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	31278	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	137.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.58% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MG, Y01, YCM, 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	0.40	0/3960	0.55	0/5387
1	C	0.40	0/3577	0.54	0/4893
1	D	0.40	0/3988	0.55	0/5443
2	B	0.39	0/4091	0.54	0/5565
3	E	0.41	0/3983	0.55	0/5429
4	F	0.40	0/4086	0.55	0/5561
4	G	0.40	0/3847	0.55	0/5243
5	H	0.40	0/3654	0.54	0/4986
All	All	0.40	0/31186	0.55	0/42507

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	3910	0	3649	23	0
1	C	3541	0	3039	9	0
1	D	3937	0	3601	15	0
2	B	4051	0	3806	19	0
3	E	3947	0	3630	18	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	4047	0	3827	27	0
4	G	3812	0	3478	17	0
5	H	3606	0	3072	16	0
6	A	27	0	12	1	0
6	B	27	0	12	0	0
6	C	27	0	12	0	0
6	D	27	0	12	1	0
6	E	27	0	12	1	0
6	F	27	0	12	1	0
6	G	27	0	12	0	0
6	H	27	0	12	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	E	1	0	0	0	0
7	F	1	0	0	0	0
7	G	1	0	0	0	0
7	H	1	0	0	0	0
8	A	30	0	36	1	0
8	B	35	0	49	1	0
8	D	26	0	32	1	0
8	E	28	0	32	1	0
8	F	35	0	49	1	0
8	G	21	0	28	1	0
8	H	28	0	32	1	0
All	All	31278	0	28456	131	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 2.

The worst 5 of 131 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:A:569:ILE:HG22	1:A:627:ILE:HD11	1.77	0.67
1:D:569:ILE:HG22	1:D:627:ILE:HD11	1.75	0.67
3:E:569:ILE:HG22	3:E:627:ILE:HD11	1.78	0.65
5:H:569:ILE:HG22	5:H:627:ILE:HD11	1.79	0.65
2:B:569:ILE:HG22	2:B:627:ILE:HD11	1.78	0.65

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	543/612 (89%)	525 (97%)	18 (3%)	0	100	100
1	C	526/612 (86%)	509 (97%)	17 (3%)	0	100	100
1	D	568/612 (93%)	550 (97%)	18 (3%)	0	100	100
2	B	567/612 (93%)	546 (96%)	21 (4%)	0	100	100
3	E	570/612 (93%)	549 (96%)	21 (4%)	0	100	100
4	F	567/612 (93%)	547 (96%)	20 (4%)	0	100	100
4	G	542/612 (89%)	524 (97%)	18 (3%)	0	100	100
5	H	538/612 (88%)	522 (97%)	16 (3%)	0	100	100
All	All	4421/4896 (90%)	4272 (97%)	149 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	359/497 (72%)	351 (98%)	8 (2%)	52	75
1	C	271/497 (54%)	266 (98%)	5 (2%)	59	79
1	D	340/497 (68%)	331 (97%)	9 (3%)	46	72
2	B	368/496 (74%)	361 (98%)	7 (2%)	57	78
3	E	344/496 (69%)	338 (98%)	6 (2%)	60	80
4	F	375/496 (76%)	363 (97%)	12 (3%)	39	67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	G	333/496 (67%)	329 (99%)	4 (1%)	71	85
5	H	280/498 (56%)	274 (98%)	6 (2%)	53	76
All	All	2670/3973 (67%)	2613 (98%)	57 (2%)	53	76

5 of 57 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	480	SER
3	E	393	THR
5	H	236	LEU
1	D	490	LEU
1	D	707	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	387	ASN
3	E	422	GLN
4	F	162	ASN
4	F	205	GLN
4	G	238	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

11 non-standard protein/DNA/RNA residues are modelled in this entry.

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
2	YCM	B	461	2	7,9,10	0.42	0	4,10,12	0.54	0
1	YCM	C	483	1	7,9,10	0.40	0	4,10,12	0.26	0
4	YCM	F	483	4	7,9,10	0.38	0	4,10,12	0.46	0
1	YCM	A	483	1	7,9,10	0.40	0	4,10,12	0.26	0
1	YCM	D	483	1	7,9,10	0.40	0	4,10,12	0.35	0
4	YCM	G	483	4	7,9,10	0.40	0	4,10,12	0.25	0
3	YCM	E	483	3	7,9,10	0.40	0	4,10,12	0.24	0
2	YCM	B	483	2	7,9,10	0.38	0	4,10,12	0.29	0
4	YCM	F	478	4	7,9,10	0.51	0	4,10,12	0.26	0
3	YCM	E	366	3	7,9,10	0.41	0	4,10,12	0.23	0
4	YCM	G	478	4	7,9,10	0.43	0	4,10,12	0.38	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	YCM	B	461	2	-	3/6/8/10	-
1	YCM	C	483	1	-	1/6/8/10	-
4	YCM	F	483	4	-	3/6/8/10	-
1	YCM	A	483	1	-	1/6/8/10	-
1	YCM	D	483	1	-	1/6/8/10	-
4	YCM	G	483	4	-	1/6/8/10	-
3	YCM	E	483	3	-	1/6/8/10	-
2	YCM	B	483	2	-	1/6/8/10	-
4	YCM	F	478	4	-	1/6/8/10	-
3	YCM	E	366	3	-	1/6/8/10	-
4	YCM	G	478	4	-	0/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	461	YCM	SG-CD-CE-OZ1
2	B	461	YCM	SG-CD-CE-NZ2
1	C	483	YCM	SG-CD-CE-NZ2
4	F	483	YCM	SG-CD-CE-OZ1
4	F	483	YCM	SG-CD-CE-NZ2

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	483	YCM	1	0
1	D	483	YCM	1	0
4	F	478	YCM	1	0
4	G	478	YCM	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 23 ligands modelled in this entry, 8 are monoatomic - leaving 15 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	$\# Z  > 2$
8	Y01	F	1003	-	35,38,38	0.33	0	54,57,57	0.43	0
6	ADP	B	1001	7	24,29,29	0.60	0	29,45,45	0.65	1 (3%)
6	ADP	A	1001	7	24,29,29	0.59	0	29,45,45	0.67	1 (3%)
6	ADP	D	1001	7	24,29,29	0.57	0	29,45,45	0.71	1 (3%)
6	ADP	C	1001	7	24,29,29	0.58	0	29,45,45	0.67	1 (3%)
6	ADP	F	1001	7	24,29,29	0.72	0	29,45,45	0.79	1 (3%)
6	ADP	E	1001	7	24,29,29	0.74	0	29,45,45	0.76	1 (3%)
6	ADP	H	1001	7	24,29,29	0.61	0	29,45,45	0.65	1 (3%)
6	ADP	G	1001	7	24,29,29	0.55	0	29,45,45	0.67	1 (3%)
8	Y01	G	1003	-	24,24,38	0.46	0	37,39,57	0.64	1 (2%)
8	Y01	E	1003	-	28,31,38	0.38	0	43,48,57	0.53	1 (2%)
8	Y01	A	1003	-	30,33,38	0.37	0	48,51,57	0.49	0
8	Y01	B	1003	-	35,38,38	0.34	0	54,57,57	0.43	0
8	Y01	H	1003	-	28,31,38	0.38	0	43,48,57	0.57	1 (2%)
8	Y01	D	1003	-	29,29,38	0.39	0	46,46,57	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	Y01	F	1003	-	-	4/17/77/77	0/4/4/4
6	ADP	B	1001	7	-	0/12/32/32	0/3/3/3
6	ADP	A	1001	7	-	0/12/32/32	0/3/3/3
6	ADP	D	1001	7	-	0/12/32/32	0/3/3/3
6	ADP	C	1001	7	-	0/12/32/32	0/3/3/3
6	ADP	F	1001	7	-	0/12/32/32	0/3/3/3
6	ADP	E	1001	7	-	0/12/32/32	0/3/3/3
6	ADP	H	1001	7	-	0/12/32/32	0/3/3/3
6	ADP	G	1001	7	-	0/12/32/32	0/3/3/3
8	Y01	G	1003	-	-	-	0/4/4/4
8	Y01	E	1003	-	-	0/7/67/77	0/4/4/4
8	Y01	A	1003	-	-	0/11/71/77	0/4/4/4
8	Y01	B	1003	-	-	5/17/77/77	0/4/4/4
8	Y01	H	1003	-	-	0/7/67/77	0/4/4/4
8	Y01	D	1003	-	-	1/8/66/77	0/4/4/4

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	1001	ADP	C5-C6-N6	2.44	124.07	120.35
8	H	1003	Y01	CBB-CBE-CBI	2.29	120.31	115.89
8	G	1003	Y01	CBB-CBE-CBI	2.28	120.28	115.89
6	C	1001	ADP	C5-C6-N6	2.27	123.80	120.35
6	A	1001	ADP	C5-C6-N6	2.27	123.80	120.35

There are no chirality outliers.

5 of 10 torsion outliers are listed below:

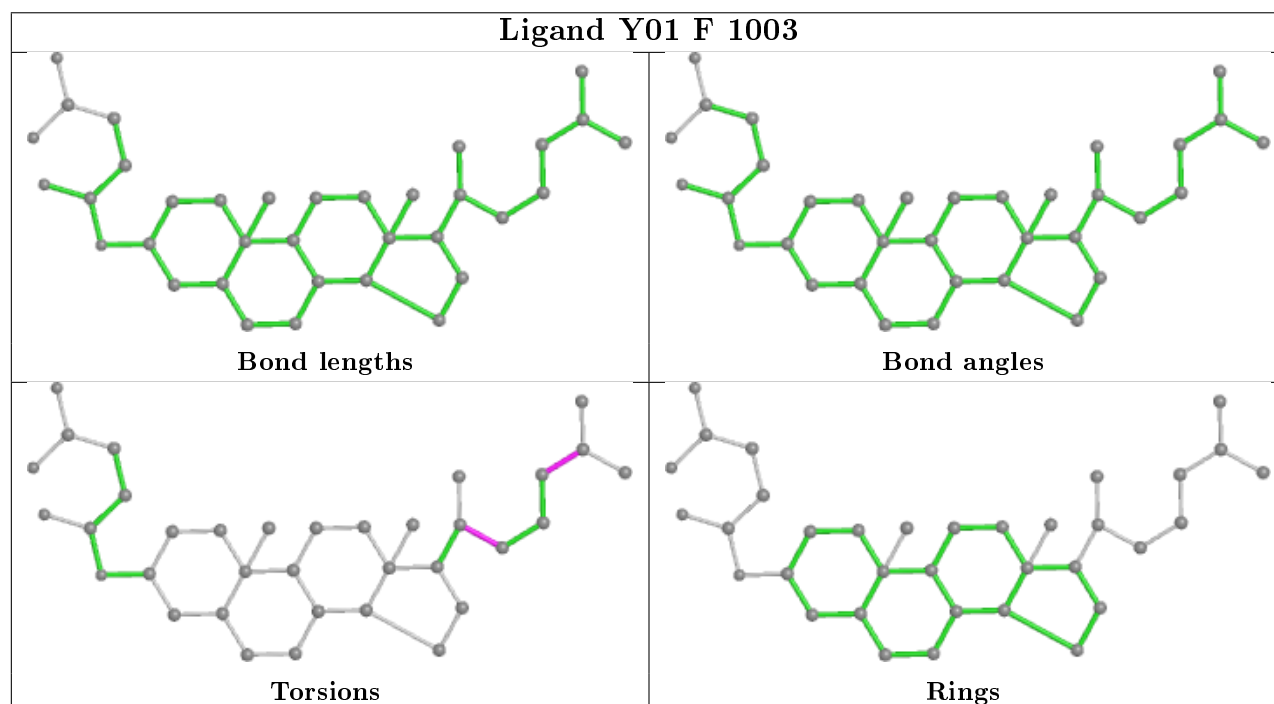
Mol	Chain	Res	Type	Atoms
8	F	1003	Y01	CAJ-CAO-CBB-CBE
8	B	1003	Y01	CAJ-CAO-CBB-CBE
8	B	1003	Y01	CAJ-CAO-CBB-CAC
8	F	1003	Y01	CAJ-CAO-CBB-CAC
8	F	1003	Y01	CAJ-CAN-CBA-CAB

There are no ring outliers.

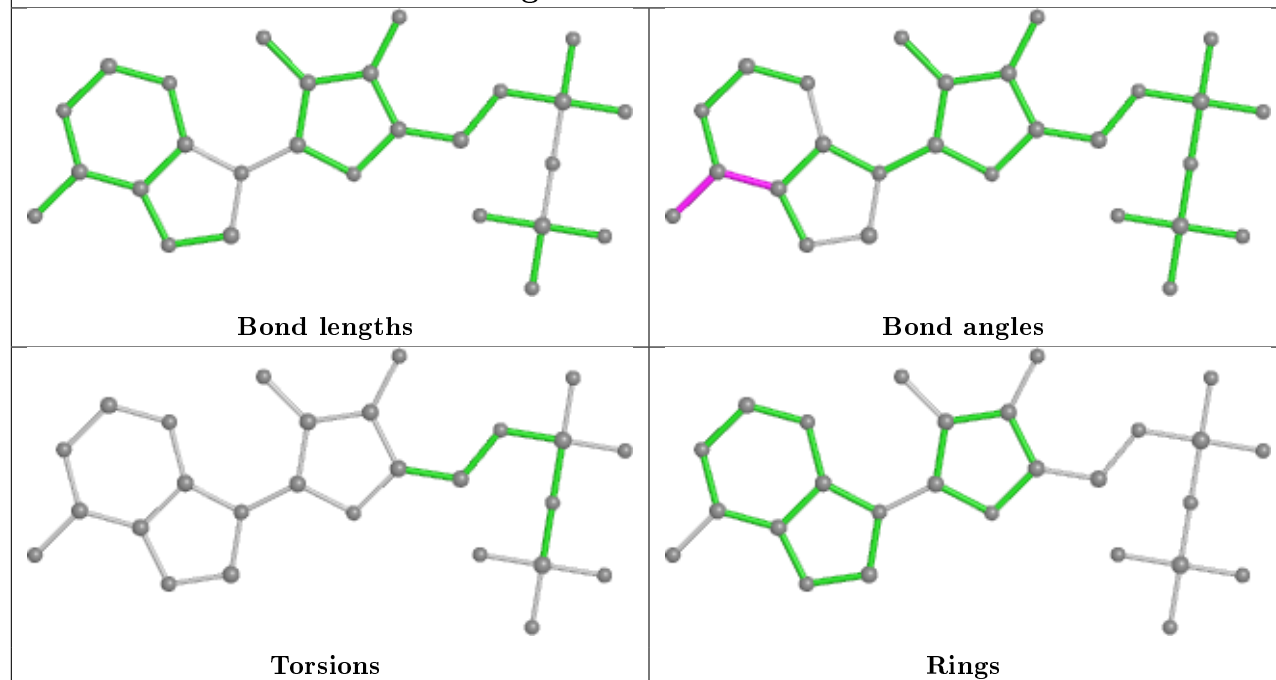
11 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	1003	Y01	1	0
6	A	1001	ADP	1	0
6	D	1001	ADP	1	0
6	F	1001	ADP	1	0
6	E	1001	ADP	1	0
8	G	1003	Y01	1	0
8	E	1003	Y01	1	0
8	A	1003	Y01	1	0
8	B	1003	Y01	1	0
8	H	1003	Y01	1	0
8	D	1003	Y01	1	0

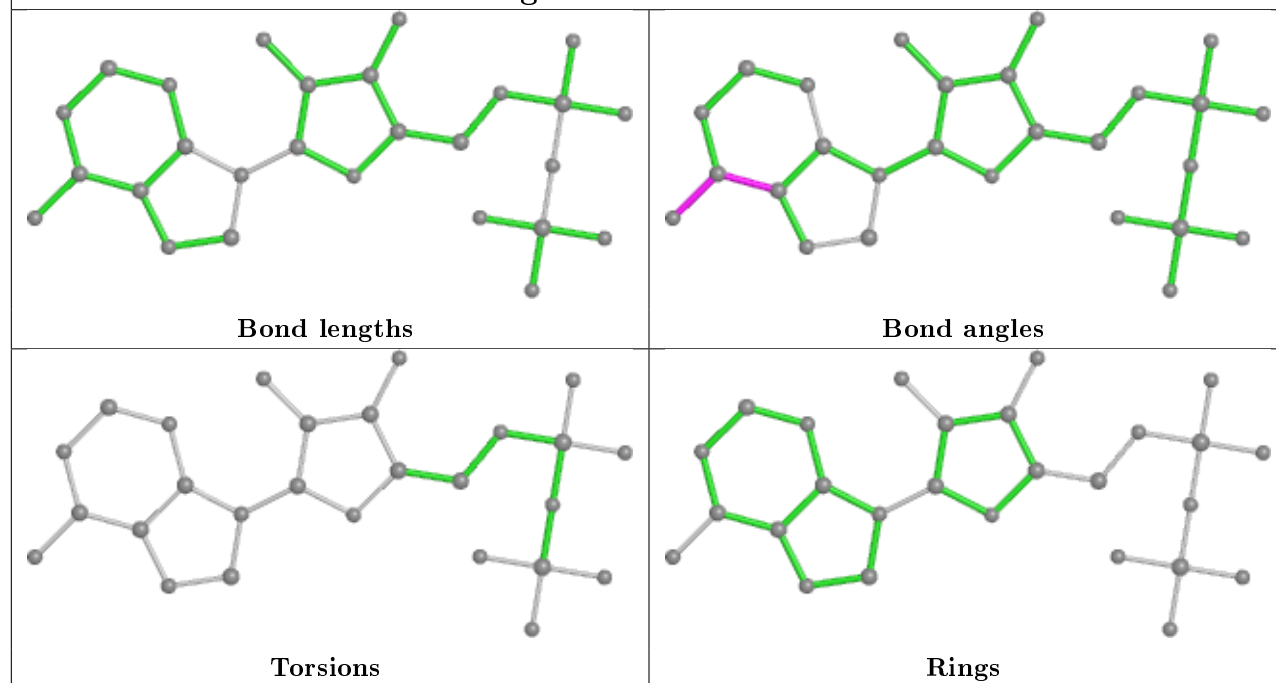
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



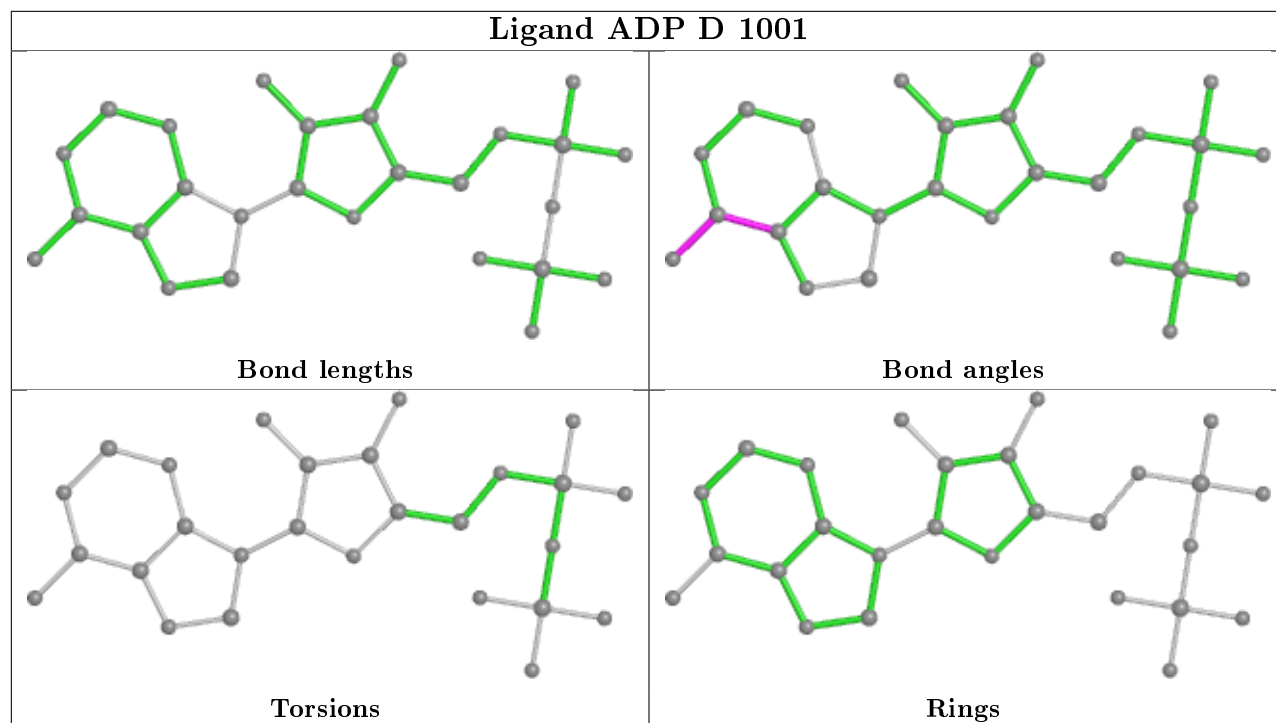
## Ligand ADP B 1001



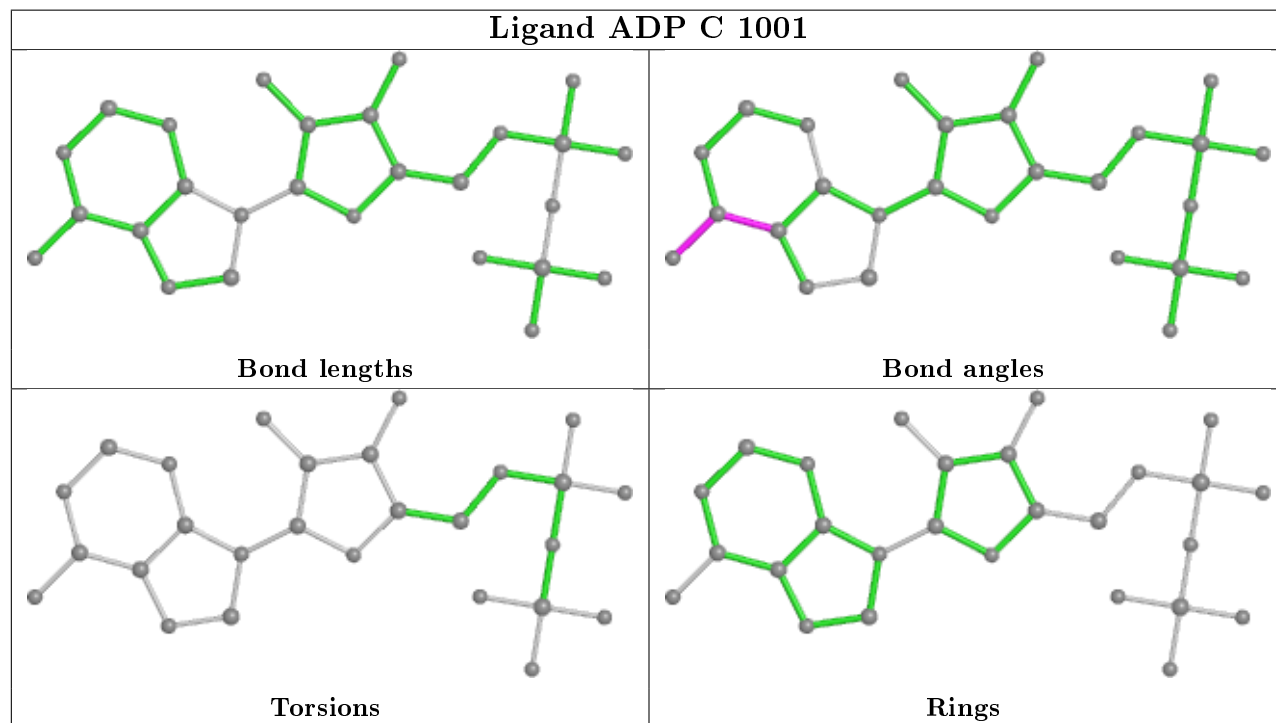
## Ligand ADP A 1001



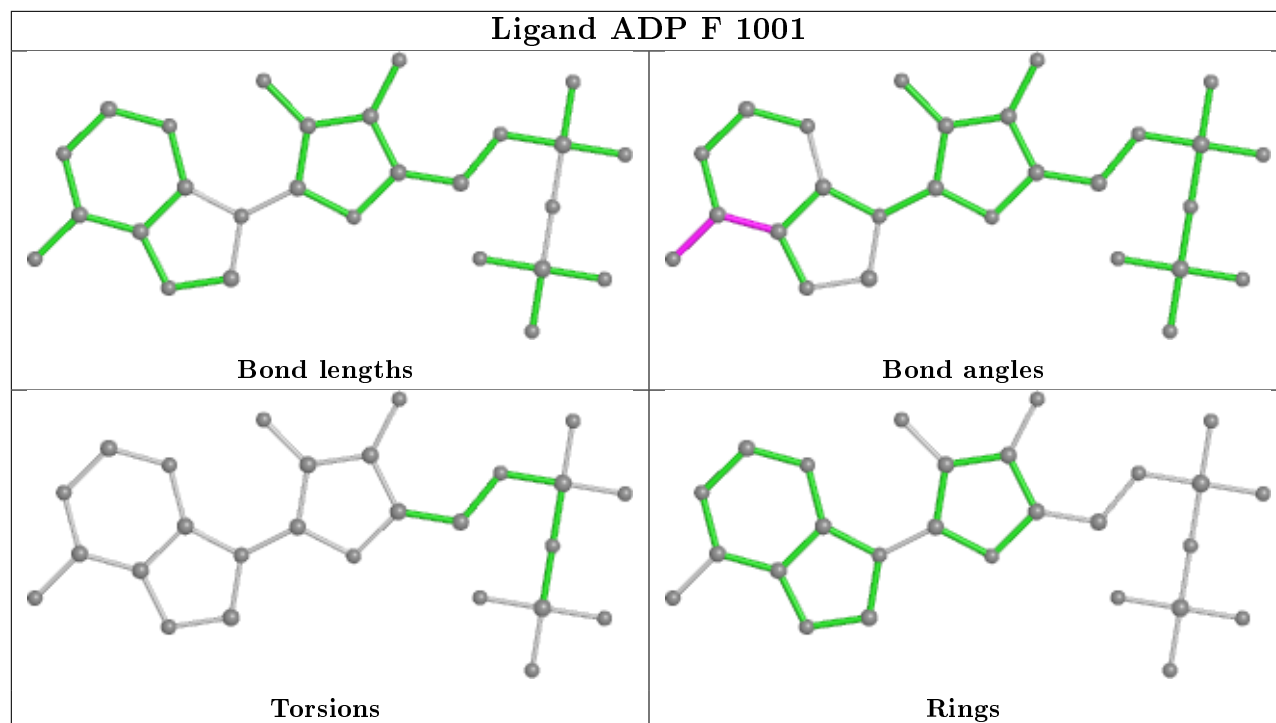
## Ligand ADP D 1001



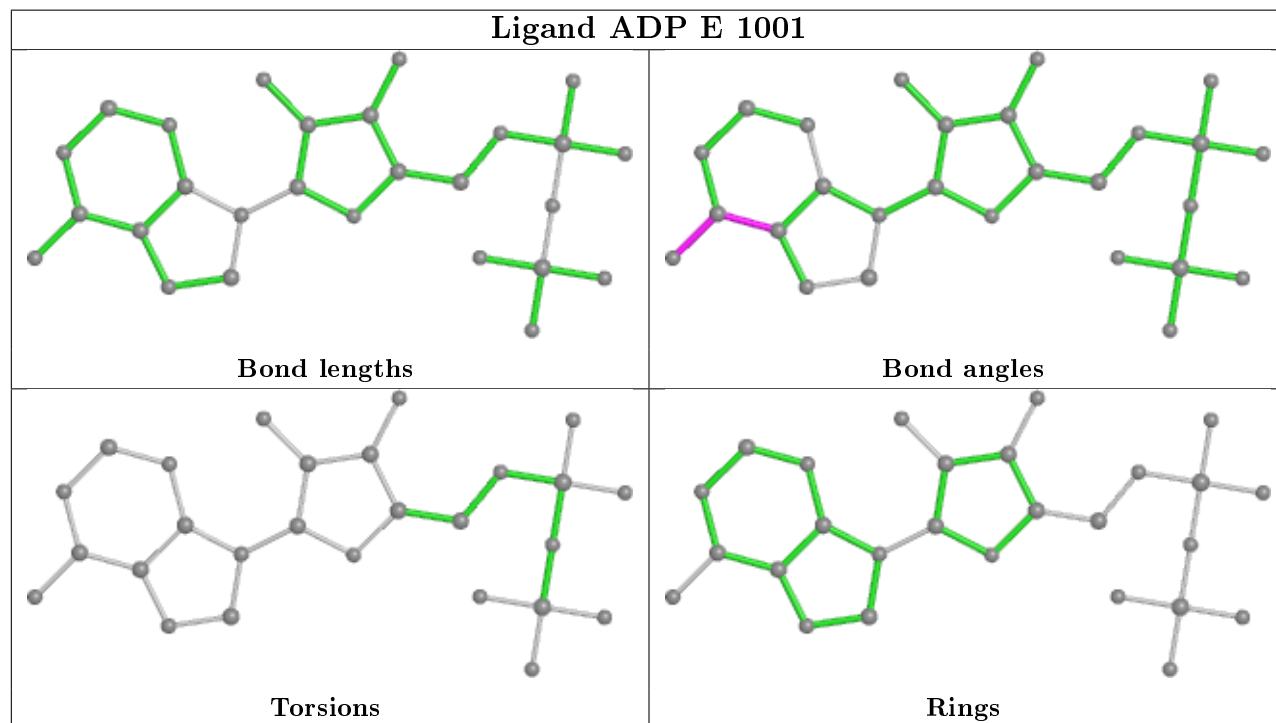
## Ligand ADP C 1001



## Ligand ADP F 1001

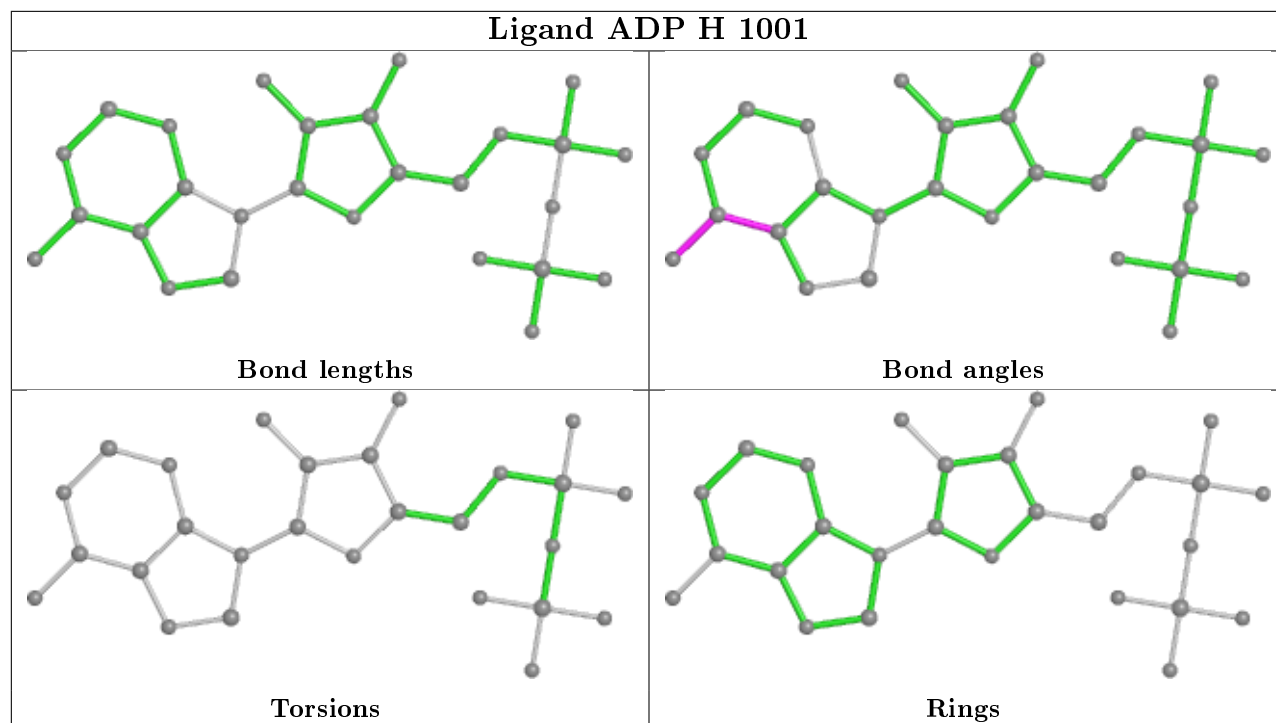


## Ligand ADP E 1001

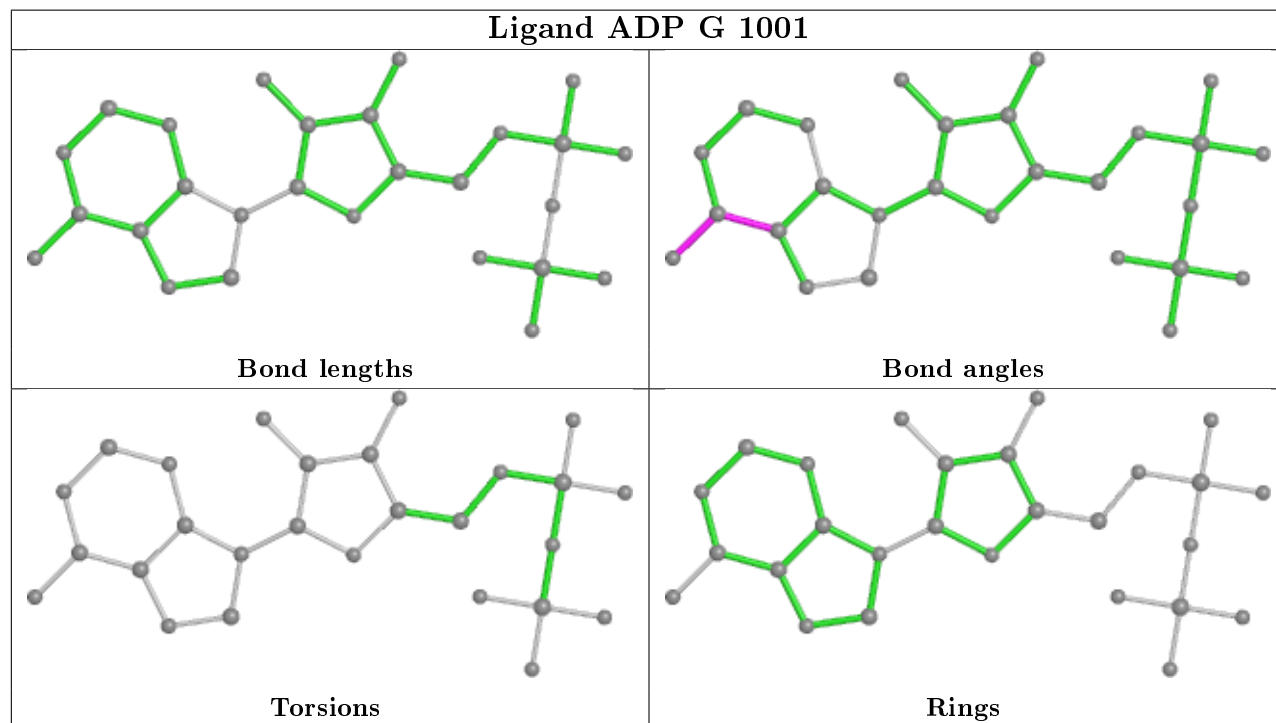


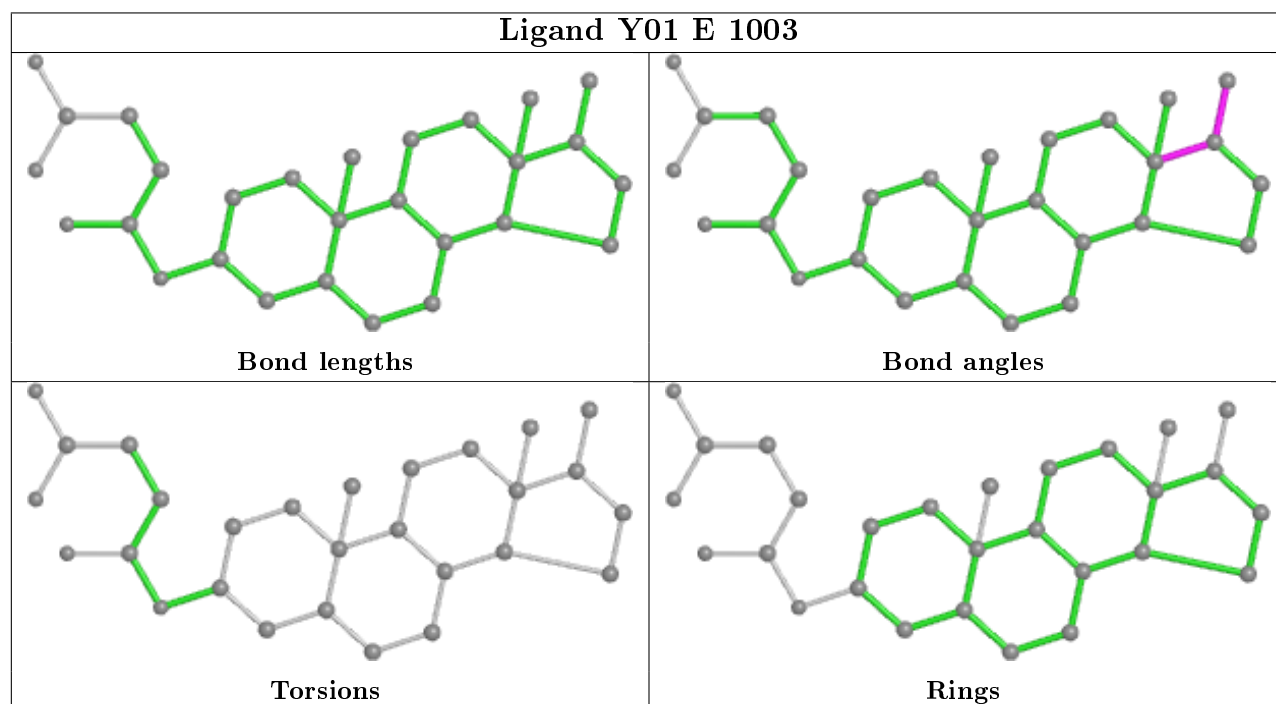
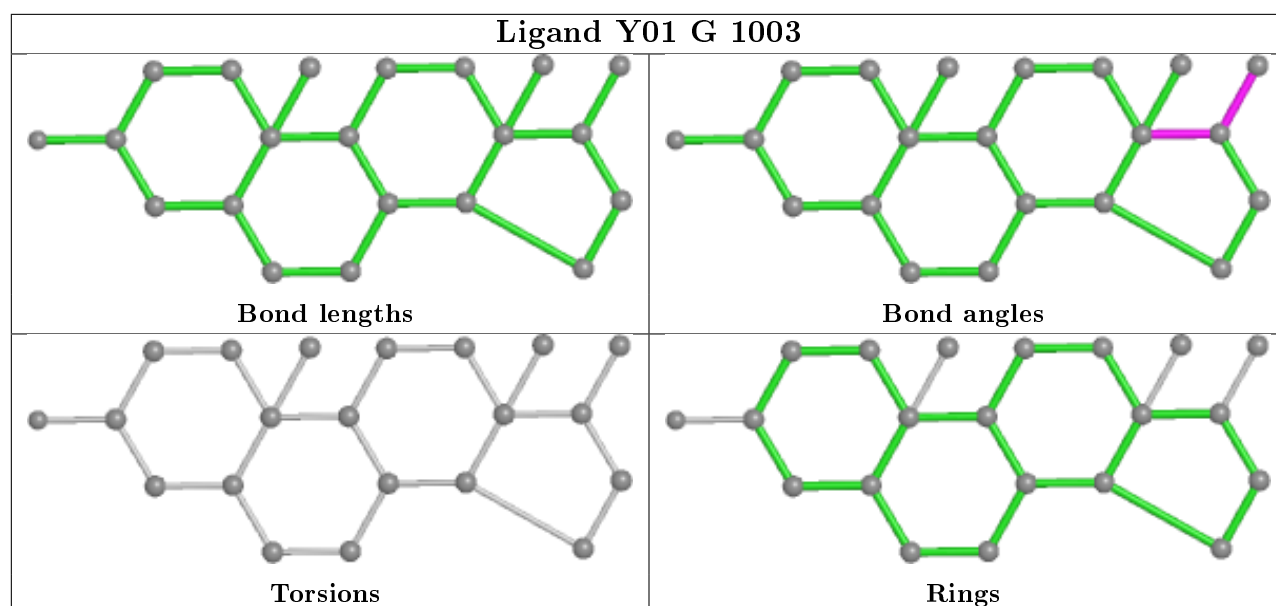


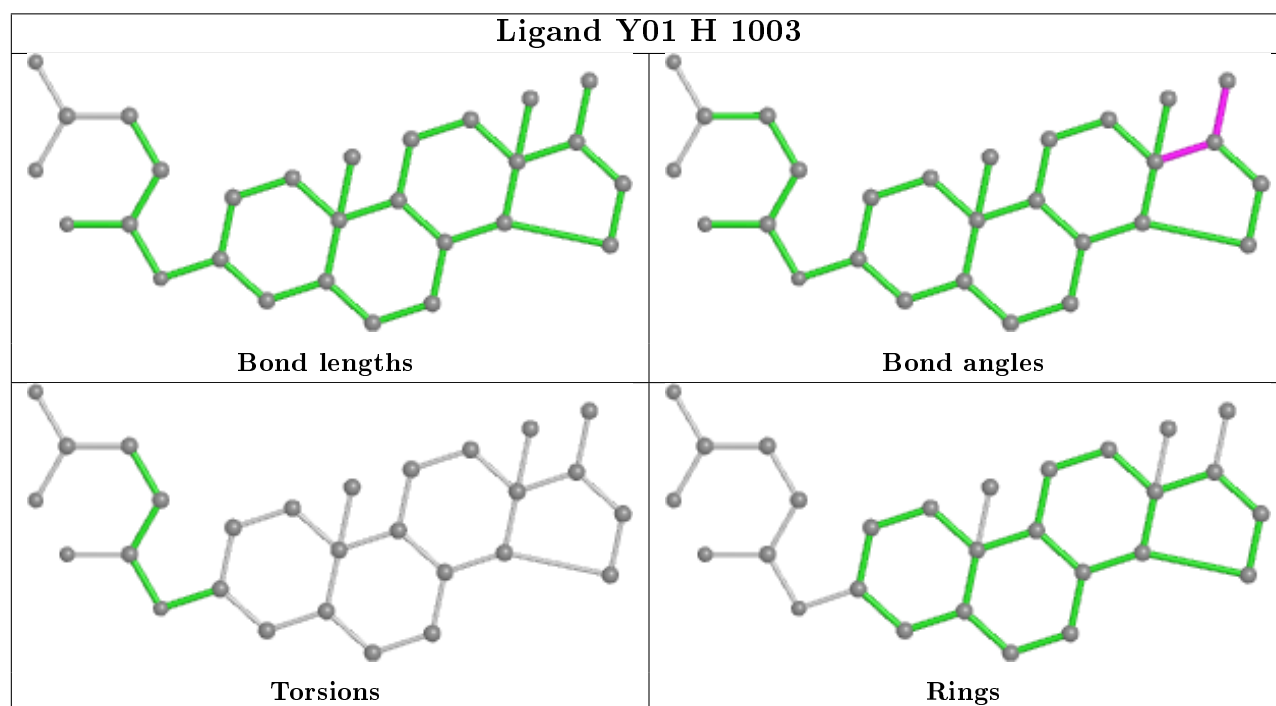
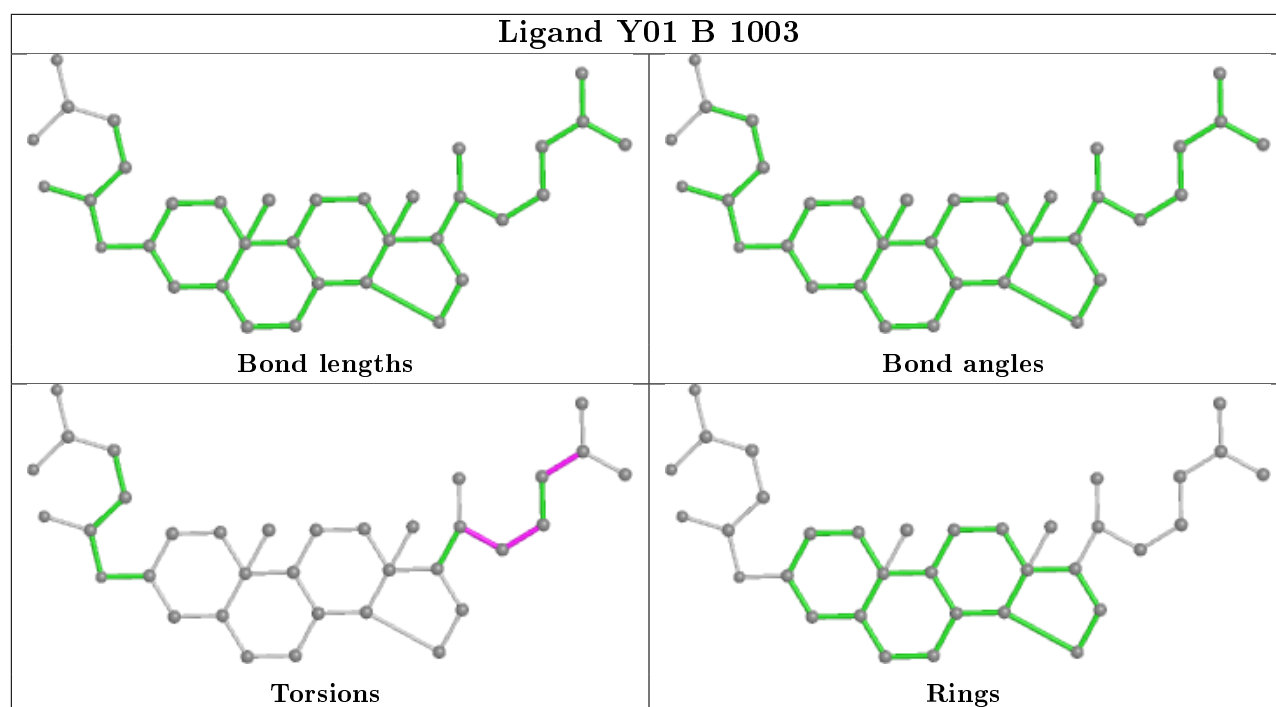
## Ligand ADP H 1001

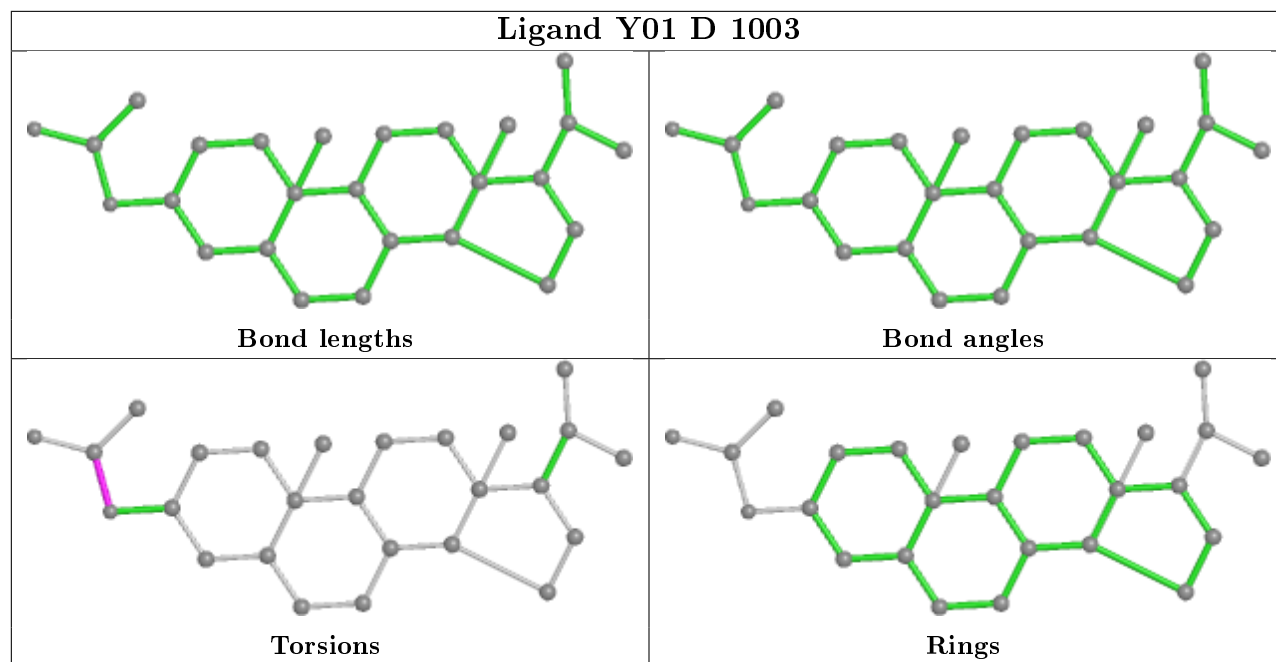


## Ligand ADP G 1001









## 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 ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	551/612 (90%)	0.07	21 (3%) 40 39	63, 111, 196, 250	0
1	C	536/612 (87%)	0.30	62 (11%) 4 5	87, 172, 227, 255	0
1	D	572/612 (93%)	0.06	29 (5%) 28 28	57, 130, 213, 239	0
2	B	571/612 (93%)	0.18	19 (3%) 46 45	46, 102, 208, 253	0
3	E	574/612 (93%)	0.41	73 (12%) 3 4	76, 161, 214, 233	0
4	F	571/612 (93%)	-0.01	16 (2%) 53 51	62, 116, 183, 204	0
4	G	550/612 (89%)	0.05	19 (3%) 44 43	74, 134, 200, 244	0
5	H	548/612 (89%)	0.32	56 (10%) 6 8	85, 173, 234, 260	0
All	All	4473/4896 (91%)	0.17	295 (6%) 18 20	46, 137, 215, 260	0

The worst 5 of 295 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	189	THR	9.0
1	C	397	GLY	8.6
3	E	632	VAL	8.5
3	E	662	THR	8.5
3	E	700	GLY	8.4

### 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	YCM	C	483	10/11	0.85	0.17	169,172,178,178	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	YCM	G	483	10/11	0.87	0.26	105,113,114,114	0
1	YCM	A	483	10/11	0.88	0.30	116,122,125,126	0
3	YCM	E	483	10/11	0.88	0.15	159,162,171,171	0
4	YCM	G	478	10/11	0.90	0.25	93,100,118,119	0
4	YCM	F	478	10/11	0.91	0.18	93,102,124,124	0
2	YCM	B	461	10/11	0.92	0.18	95,104,116,116	0
1	YCM	D	483	10/11	0.92	0.21	95,99,104,106	0
2	YCM	B	483	10/11	0.93	0.19	83,85,91,93	0
3	YCM	E	366	10/11	0.94	0.17	101,111,126,129	0
4	YCM	F	483	10/11	0.97	0.17	96,99,105,107	0

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

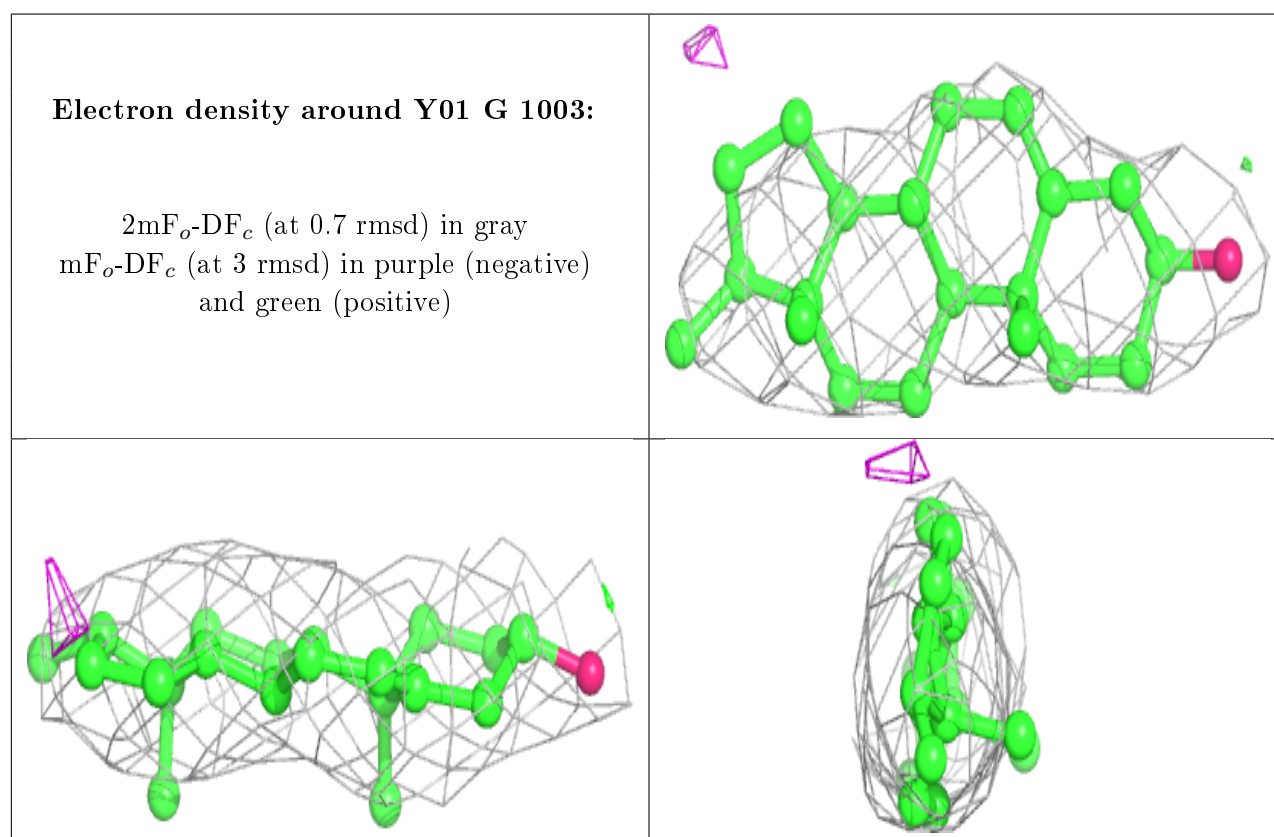
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
8	Y01	G	1003	21/35	0.87	0.56	117,119,120,120	0
6	ADP	H	1001	27/27	0.88	0.24	195,196,201,201	0
8	Y01	B	1003	35/35	0.90	0.29	109,116,129,130	0
6	ADP	C	1001	27/27	0.91	0.17	151,160,165,166	0
6	ADP	E	1001	27/27	0.92	0.26	144,153,160,160	0
8	Y01	D	1003	26/35	0.92	0.27	110,114,118,118	0
6	ADP	D	1001	27/27	0.93	0.20	102,106,110,112	0
7	MG	D	1002	1/1	0.93	0.26	48,48,48,48	0
7	MG	H	1002	1/1	0.94	0.10	99,99,99,99	0
6	ADP	G	1001	27/27	0.94	0.24	124,132,136,136	0
8	Y01	E	1003	28/35	0.94	0.34	102,106,116,117	0
6	ADP	A	1001	27/27	0.95	0.21	94,105,114,114	0
7	MG	C	1002	1/1	0.95	0.10	97,97,97,97	0
6	ADP	F	1001	27/27	0.95	0.15	108,113,118,119	0
8	Y01	A	1003	30/35	0.95	0.27	96,101,115,116	0
7	MG	G	1002	1/1	0.96	0.09	75,75,75,75	0
8	Y01	F	1003	35/35	0.96	0.29	76,80,93,95	0
8	Y01	H	1003	28/35	0.96	0.23	96,100,110,112	0

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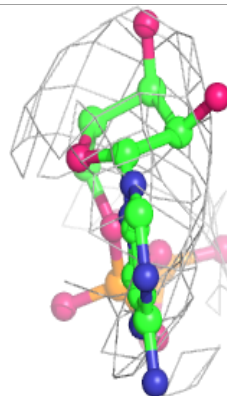
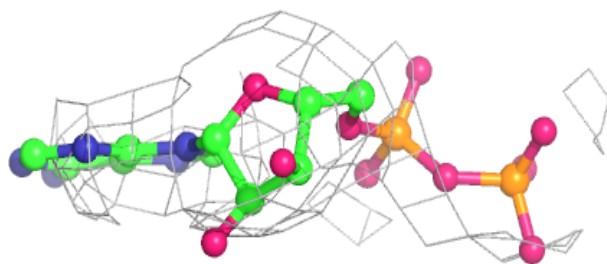
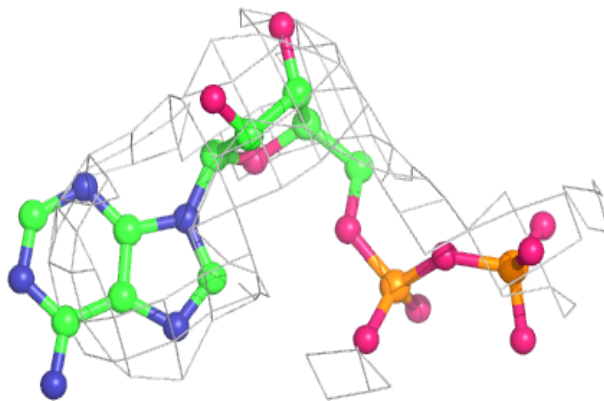
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	ADP	B	1001	27/27	0.97	0.20	92,100,104,104	0
7	MG	F	1002	1/1	0.98	0.21	52,52,52,52	0
7	MG	B	1002	1/1	0.98	0.16	34,34,34,34	0
7	MG	E	1002	1/1	0.98	0.13	109,109,109,109	0
7	MG	A	1002	1/1	0.99	0.16	51,51,51,51	0

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.

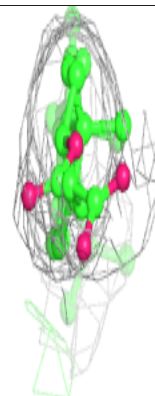
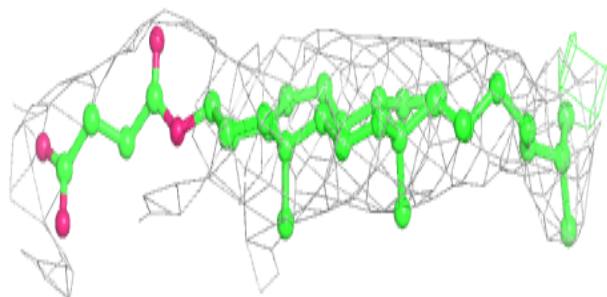
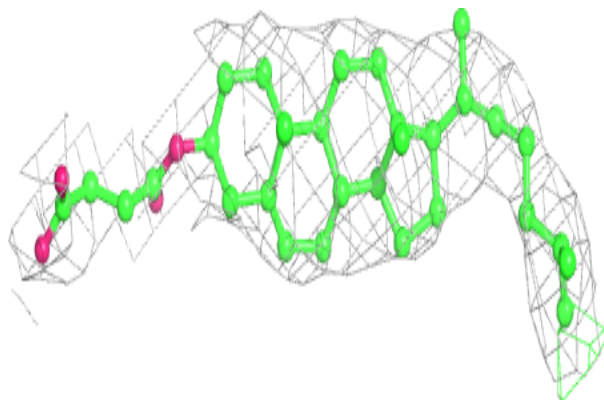


**Electron density around ADP H 1001:**

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

**Electron density around Y01 B 1003:**

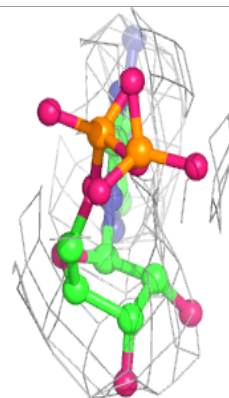
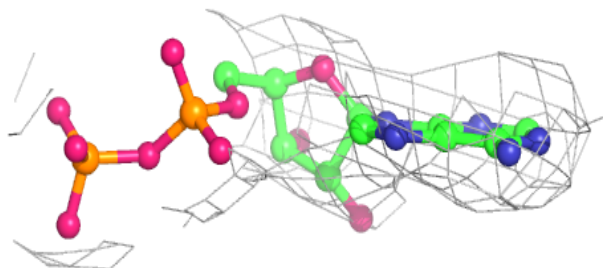
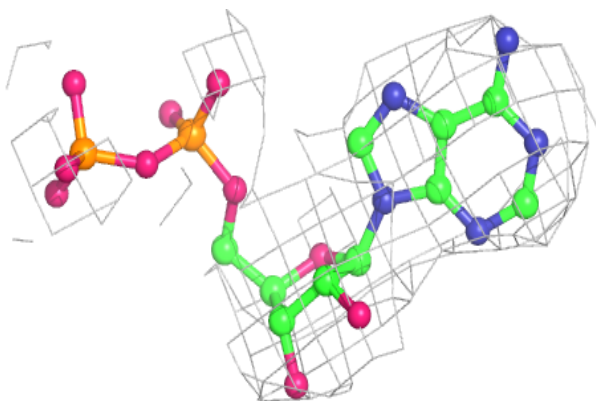
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



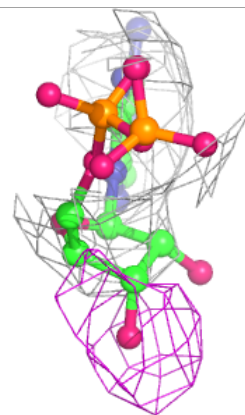
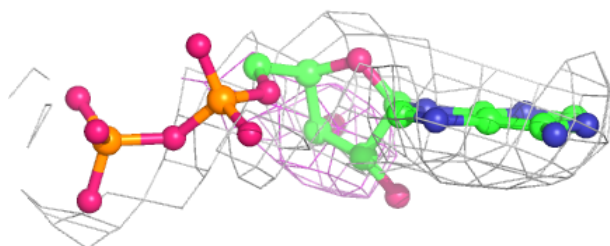
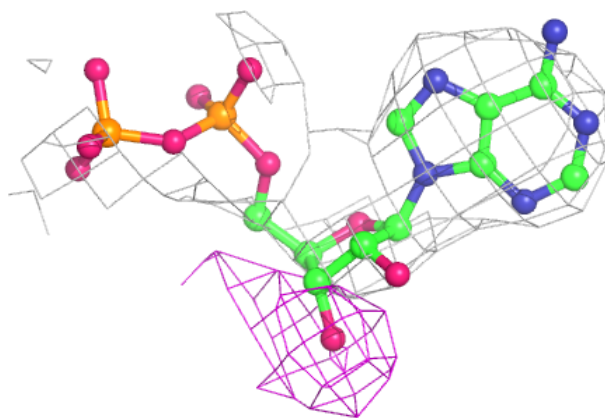


**Electron density around ADP C 1001:**

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

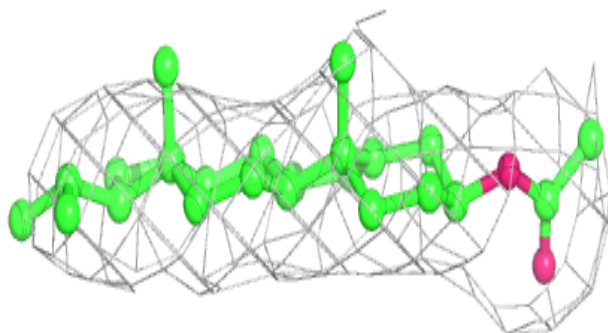
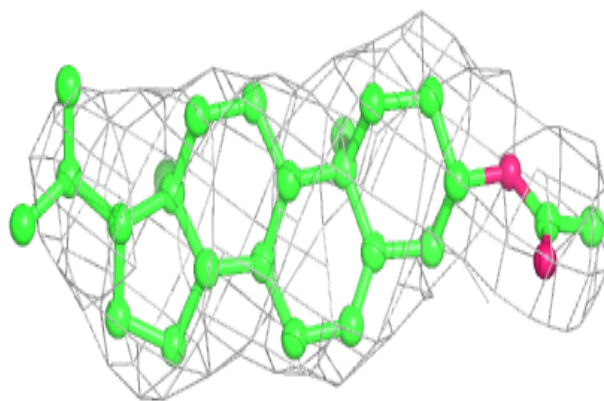
**Electron density around ADP E 1001:**

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

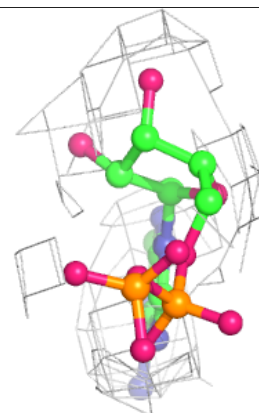
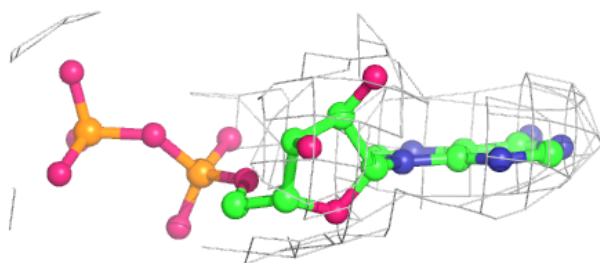
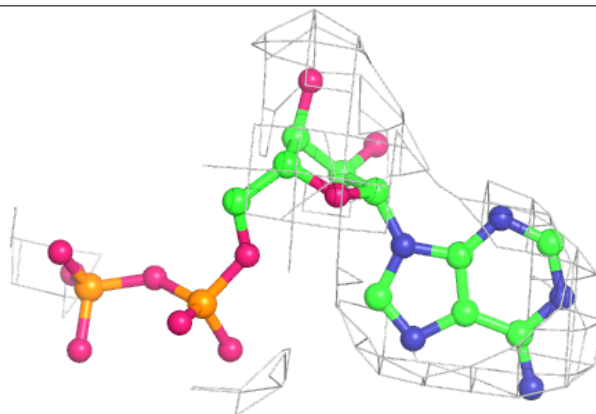


**Electron density around Y01 D 1003:**

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

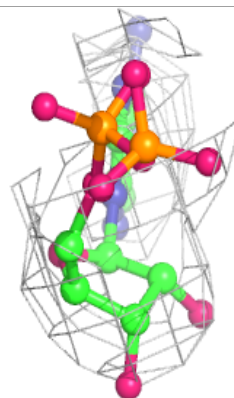
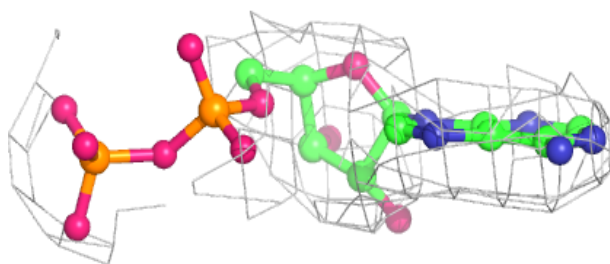
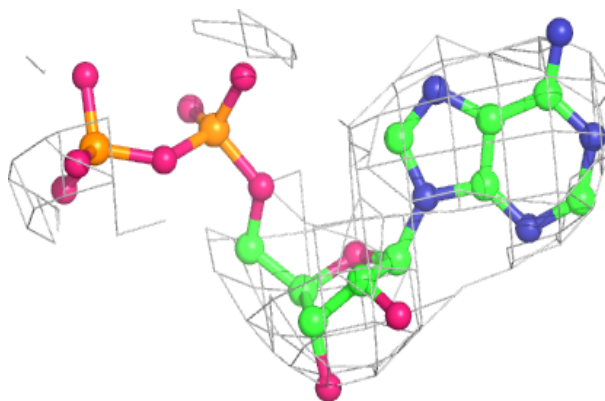
**Electron density around ADP D 1001:**

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

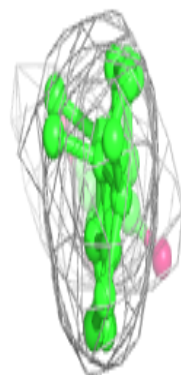
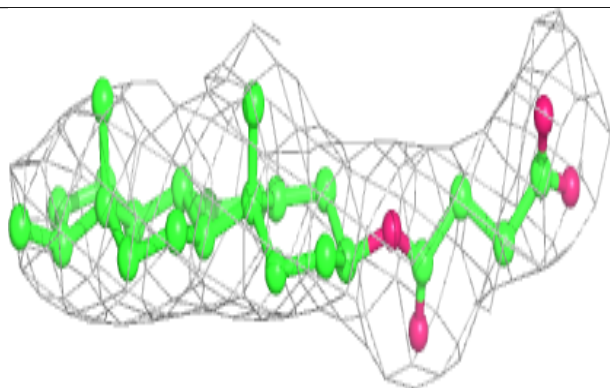
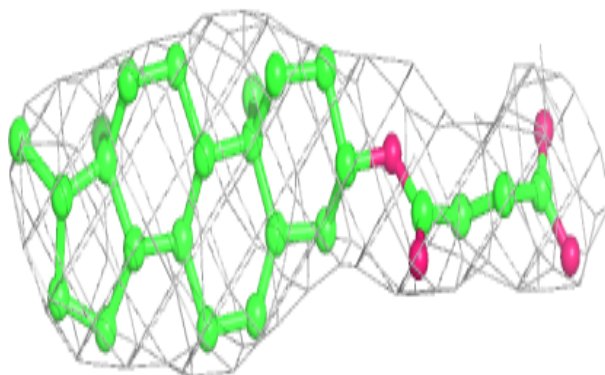


**Electron density around ADP G 1001:**

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

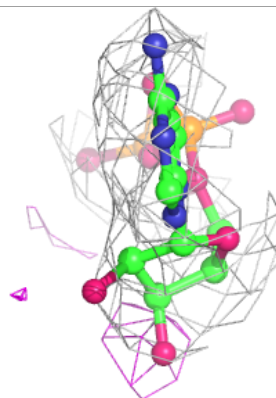
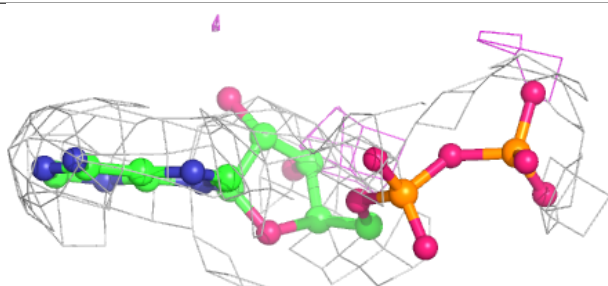
**Electron density around Y01 E 1003:**

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

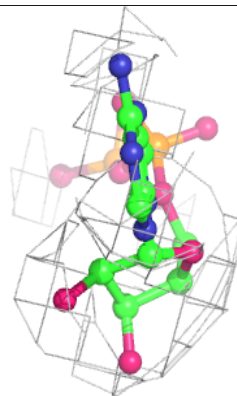
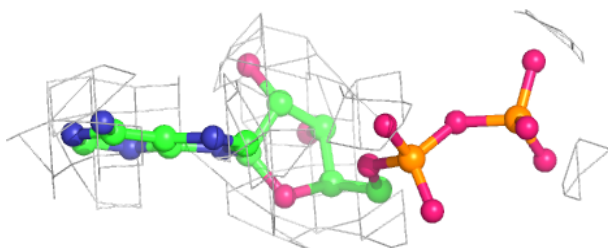
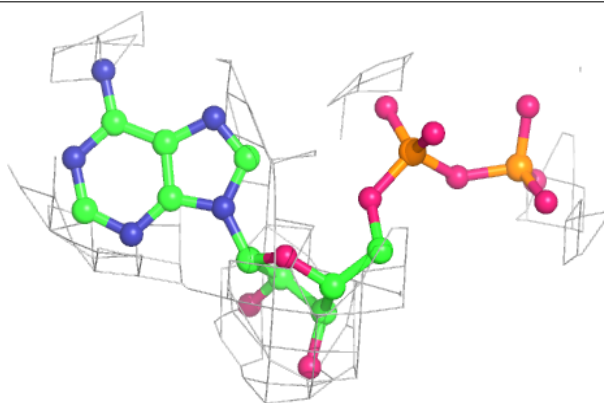


**Electron density around ADP A 1001:**

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

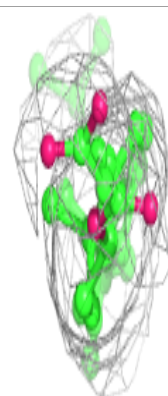
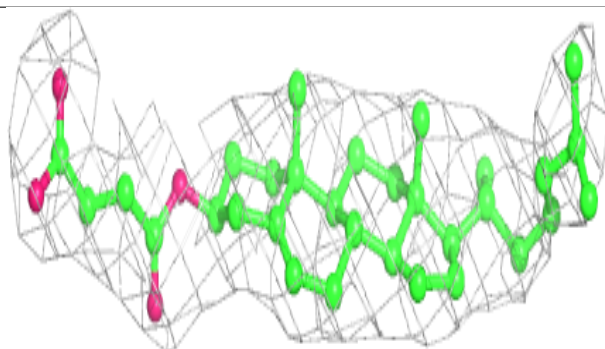
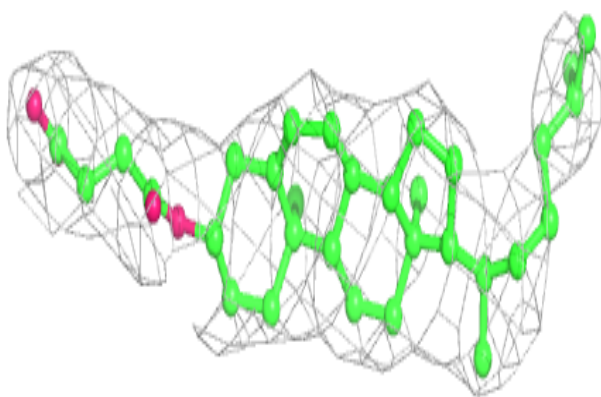
**Electron density around ADP F 1001:**

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

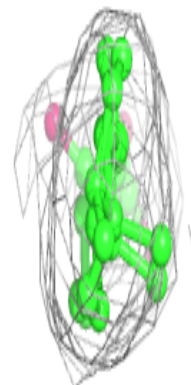
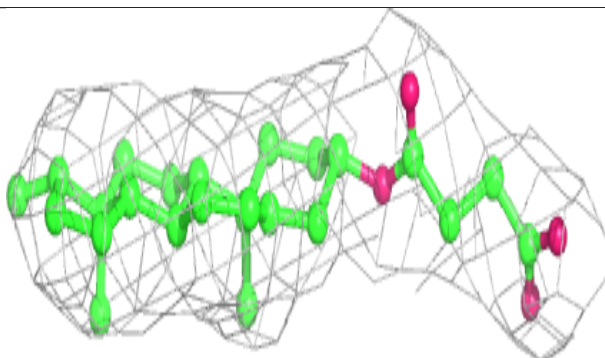
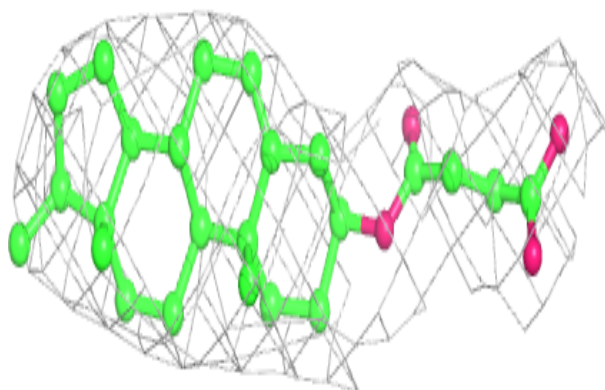


**Electron density around Y01 F 1003:**

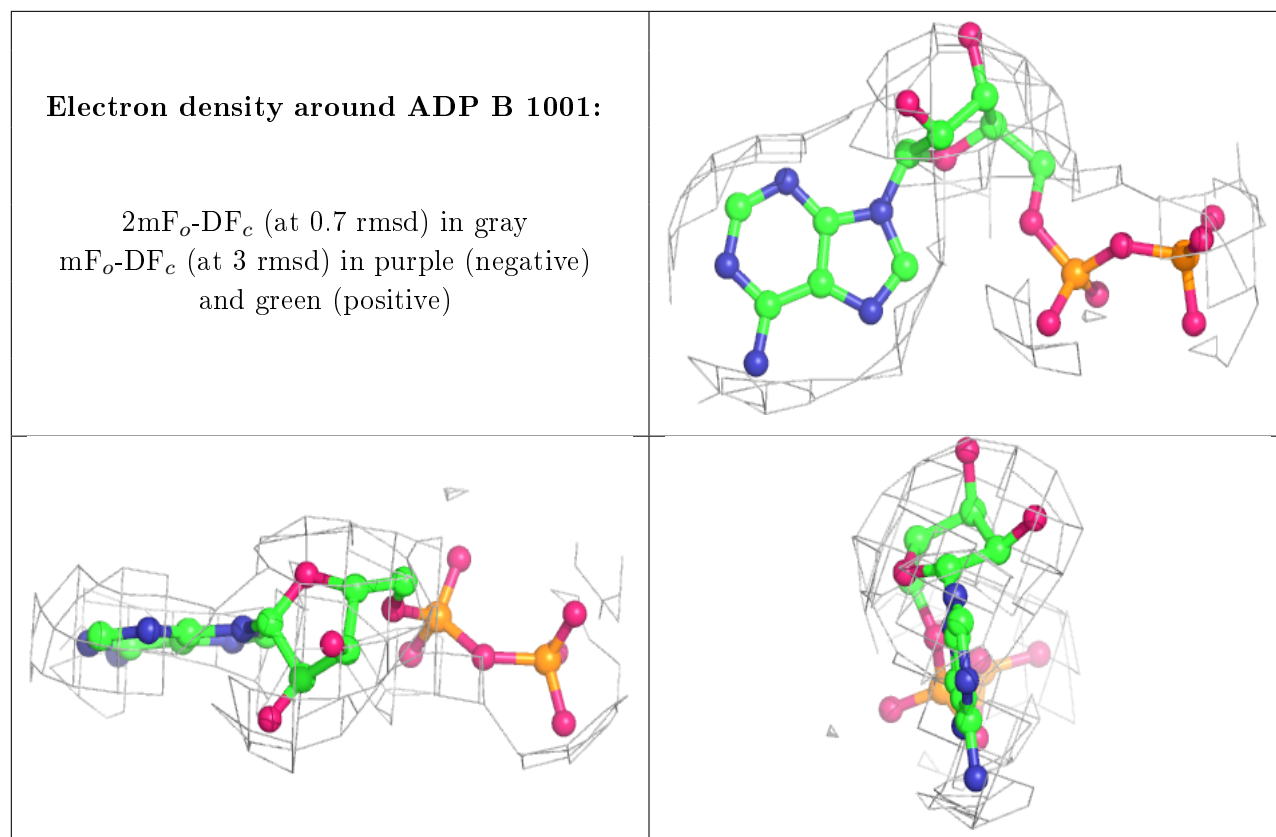
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

**Electron density around Y01 H 1003:**

$2mF_o-DF_c$  (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.