wwPDB X-ray Structure Validation Summary Report (i)

Dec 17, 2023 – 11:34 AM EST

PDB ID	:	4PKN
Title	:	Crystal structure of the football-shaped GroEL-GroES2-(ADPBeFx)14 complex containing substrate Rubisco
Authors	:	Fei, X.; Ye, X.; Laronde-Leblanc, N.; Lorimer, G.H.
Deposited on	:	2014-05-15
Resolution	:	3.66 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

The following versions of software and data (see references (1)) were used in the production of this report:

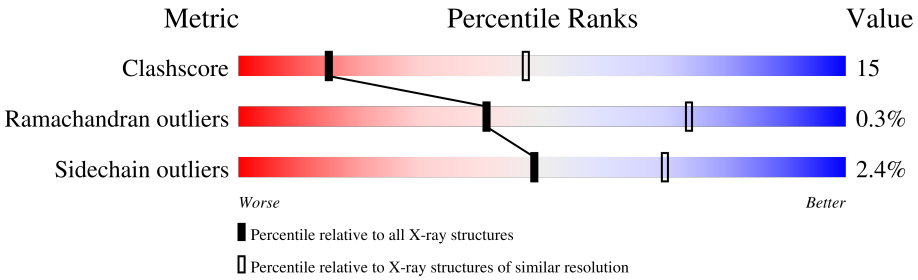
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	FAILED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.66 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))
Clashscore	141614	1037 (3.80-3.52)
Ramachandran outliers	138981	1004 (3.80-3.52)
Sidechain outliers	138945	1002 (3.80-3.52)

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%

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	548	70% 25% .
1	B	548	69% 26% .
1	C	548	66% 29% . .
1	D	548	70% 25% .
1	E	548	66% 29% . .
1	F	548	71% 24% . .
1	G	548	69% 26% .
1	H	548	66% 28% . .

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Mol	Chain	Length	Quality of chain
1	I	548	66% 30%
1	J	548	65% 30%
1	K	548	65% 30%
1	L	548	68% 26%
1	M	548	66% 28%
1	N	548	70% 24%
2	1	97	57% 39%
2	2	97	60% 36%
2	O	97	69% 29%
2	P	97	58% 39%
2	Q	97	57% 42%
2	R	97	63% 32% 5%
2	S	97	53% 37% 8%
2	T	97	57% 41%
2	U	97	58% 38%
2	V	97	63% 35%
2	W	97	54% 42%
2	X	97	61% 33%
2	Y	97	62% 37%
2	Z	97	57% 39%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BEF	B	602	-	-	X	-
4	BEF	E	602	-	-	X	-
4	BEF	G	602	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BEF	J	602	-	-	X	-
4	BEF	K	602	-	-	X	-
4	BEF	L	602	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 64579 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.

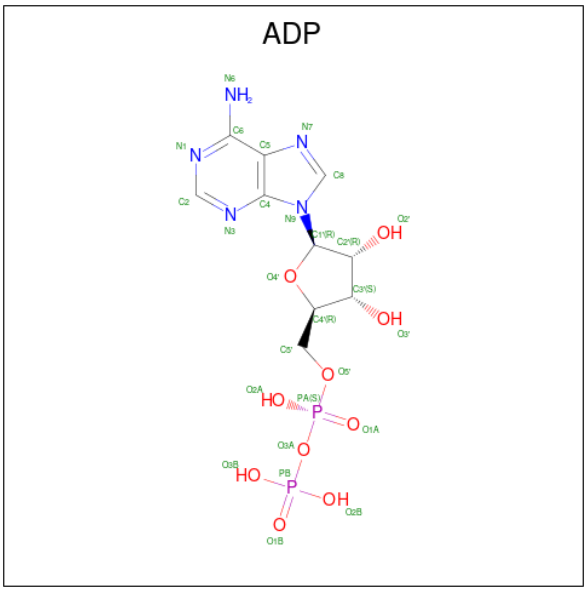
- Molecule 1 is a protein called 60 kDa chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	G	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	A	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	B	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	F	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	E	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	C	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	D	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	K	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	J	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	I	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	L	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	M	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	H	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0
1	N	524	Total 3855	C 2397	N 665	O 773	S 20	0	0	0

- Molecule 2 is a protein called 10 kDa chaperonin.

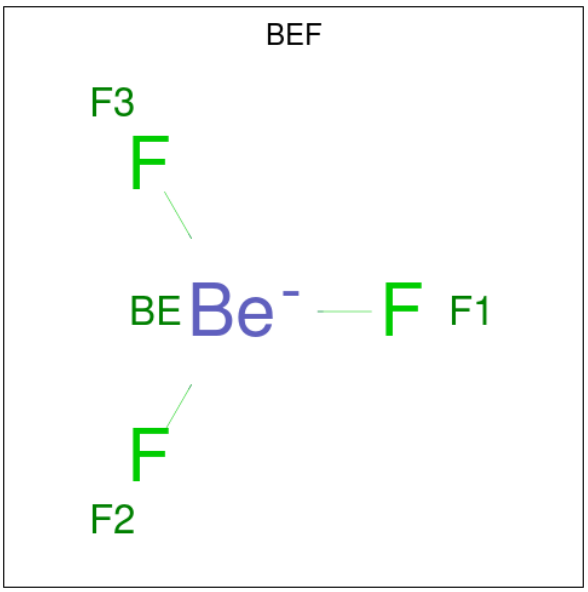
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	P	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	Q	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	U	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	T	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	R	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	S	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	X	95	Total	C	N	O	S	0	0	0
			714	446	125	142	1			
2	W	96	Total	C	N	O	S	0	0	0
			719	449	126	143	1			
2	V	96	Total	C	N	O	S	0	0	0
			722	451	126	143	2			
2	Y	96	Total	C	N	O	S	0	0	0
			722	451	126	143	2			
2	Z	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	2	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			
2	1	97	Total	C	N	O	S	0	0	0
			727	454	127	144	2			

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	G	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	K	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	J	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	I	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	L	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	M	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	N	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Be F 4 1 3	0	0
4	A	1	Total Be F 4 1 3	0	0
4	B	1	Total Be F 4 1 3	0	0
4	F	1	Total Be F 4 1 3	0	0
4	E	1	Total Be F 4 1 3	0	0
4	C	1	Total Be F 4 1 3	0	0
4	D	1	Total Be F 4 1 3	0	0
4	K	1	Total Be F 4 1 3	0	0
4	J	1	Total Be F 4 1 3	0	0
4	I	1	Total Be F 4 1 3	0	0
4	L	1	Total Be F 4 1 3	0	0
4	M	1	Total Be F 4 1 3	0	0
4	H	1	Total Be F 4 1 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	N	1	Total Be F 4 1 3	0	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	G	1	Total Mg 1 1	0	0
5	A	1	Total Mg 1 1	0	0
5	B	1	Total Mg 1 1	0	0
5	F	1	Total Mg 1 1	0	0
5	E	1	Total Mg 1 1	0	0
5	C	1	Total Mg 1 1	0	0
5	D	1	Total Mg 1 1	0	0
5	K	1	Total Mg 1 1	0	0
5	J	1	Total Mg 1 1	0	0
5	I	1	Total Mg 1 1	0	0
5	L	1	Total Mg 1 1	0	0
5	M	1	Total Mg 1 1	0	0
5	H	1	Total Mg 1 1	0	0
5	N	1	Total Mg 1 1	0	0

- Molecule 6 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	G	1	Total K 1 1	0	0
6	A	1	Total K 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total K 1 1	0	0
6	F	1	Total K 1 1	0	0
6	E	1	Total K 1 1	0	0
6	C	1	Total K 1 1	0	0
6	D	1	Total K 1 1	0	0
6	K	1	Total K 1 1	0	0
6	J	1	Total K 1 1	0	0
6	I	1	Total K 1 1	0	0
6	L	1	Total K 1 1	0	0
6	M	1	Total K 1 1	0	0
6	H	1	Total K 1 1	0	0
6	N	1	Total K 1 1	0	0

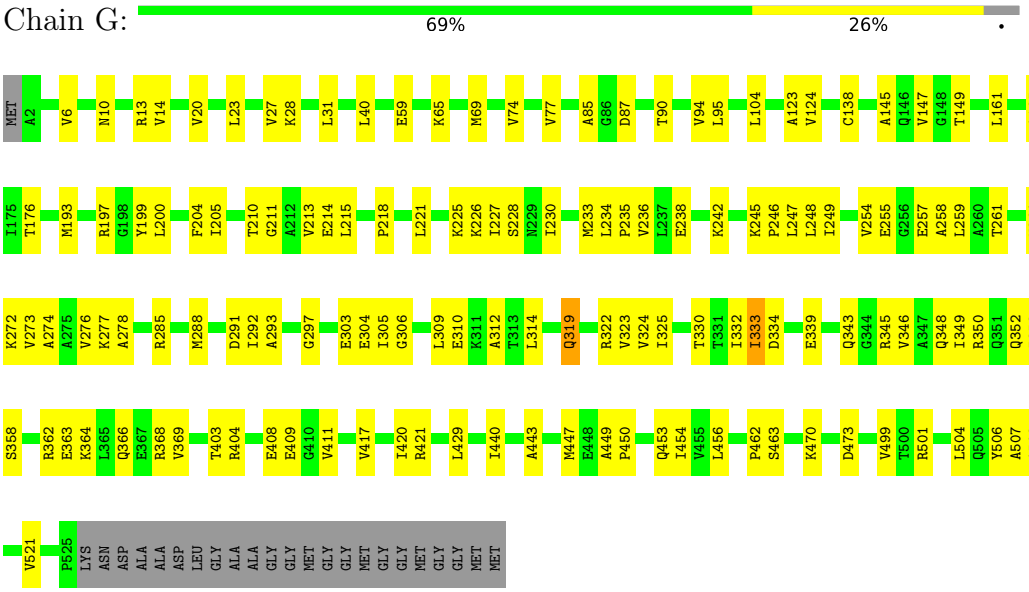
3 Residue-property plots (i)

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

Note EDS failed to run properly.

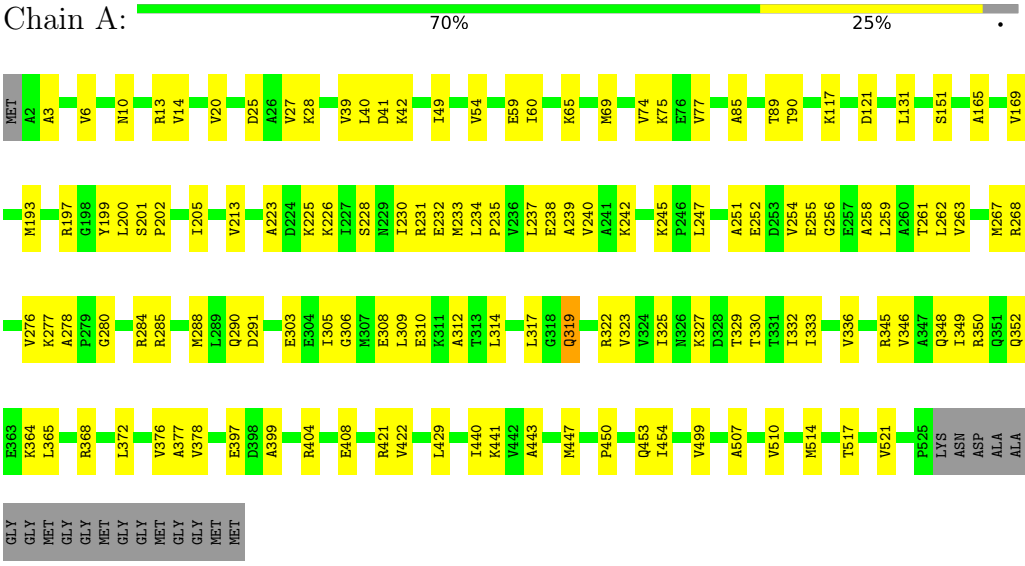
- Molecule 1: 60 kDa chaperonin

Chain G:



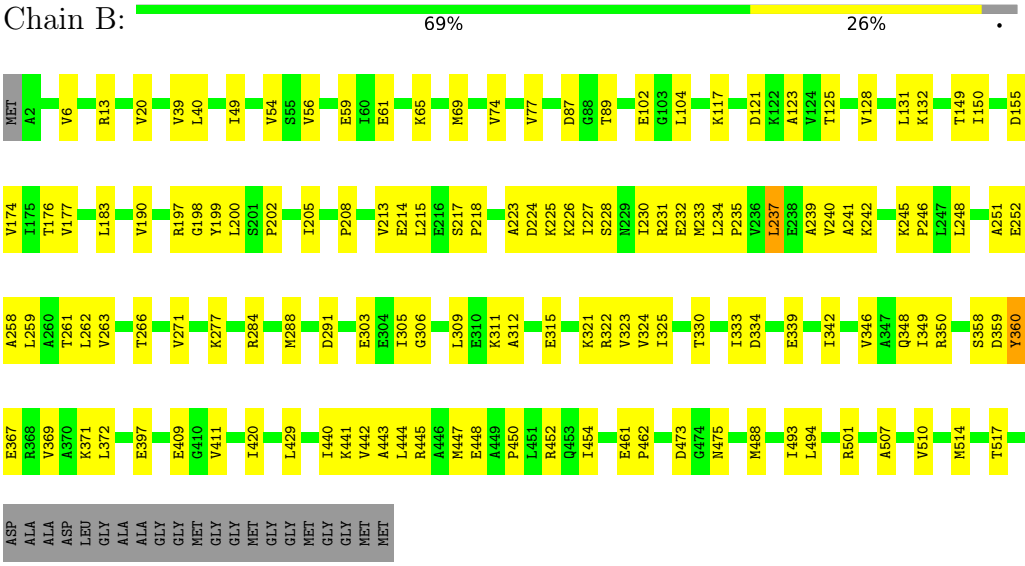
- Molecule 1: 60 kDa chaperonin

Chain A:



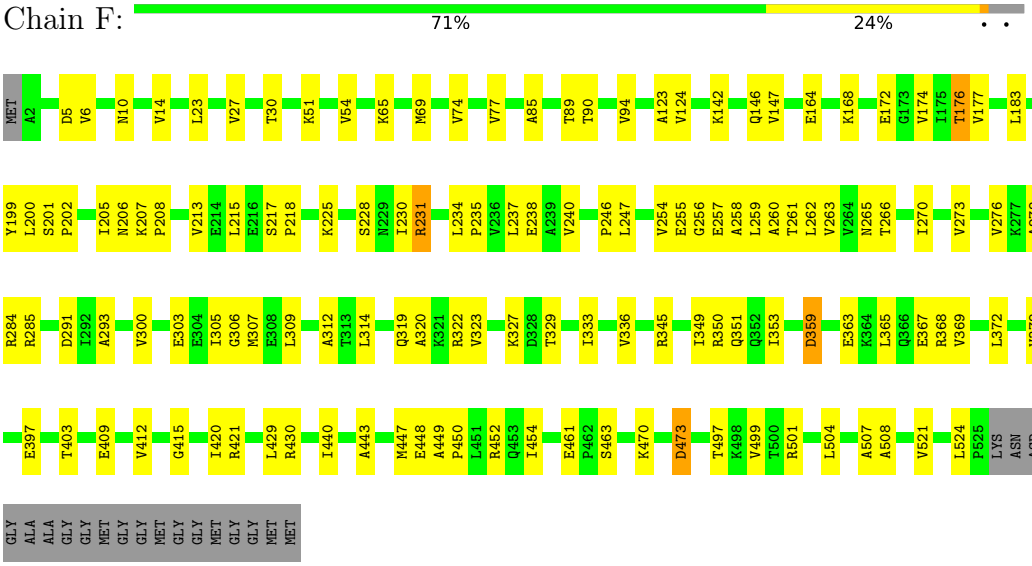
• Molecule 1: 60 kDa chaperonin

Chain B:



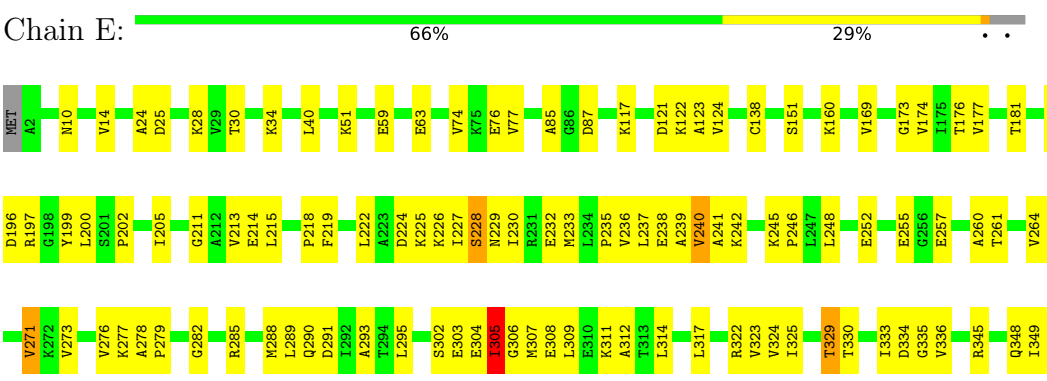
• Molecule 1: 60 kDa chaperonin

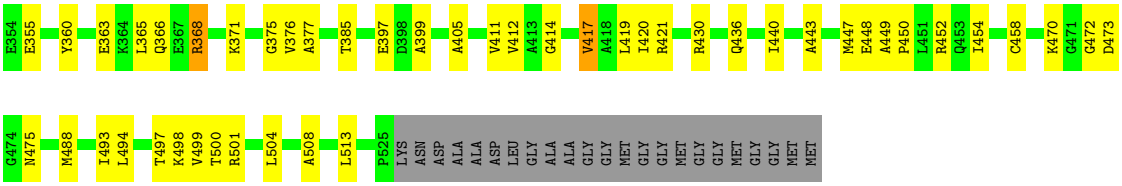
Chain F:



• Molecule 1: 60 kDa chaperonin

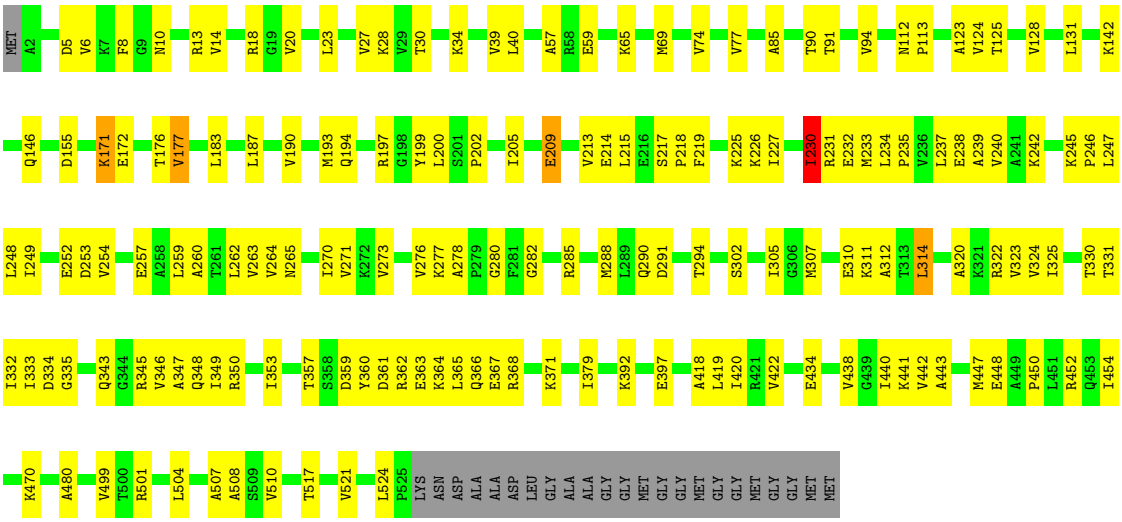
Chain E:





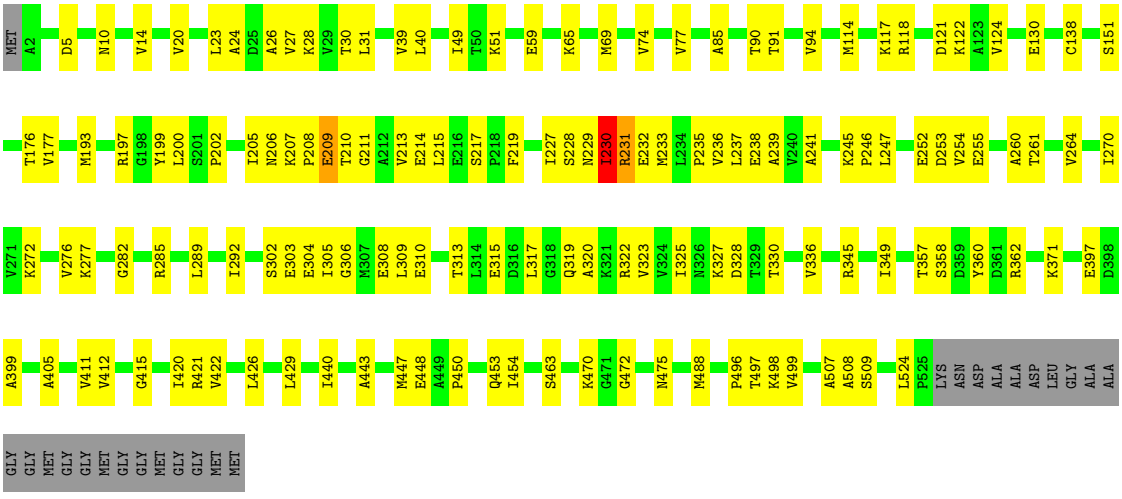
• Molecule 1: 60 kDa chaperonin

Chain C:



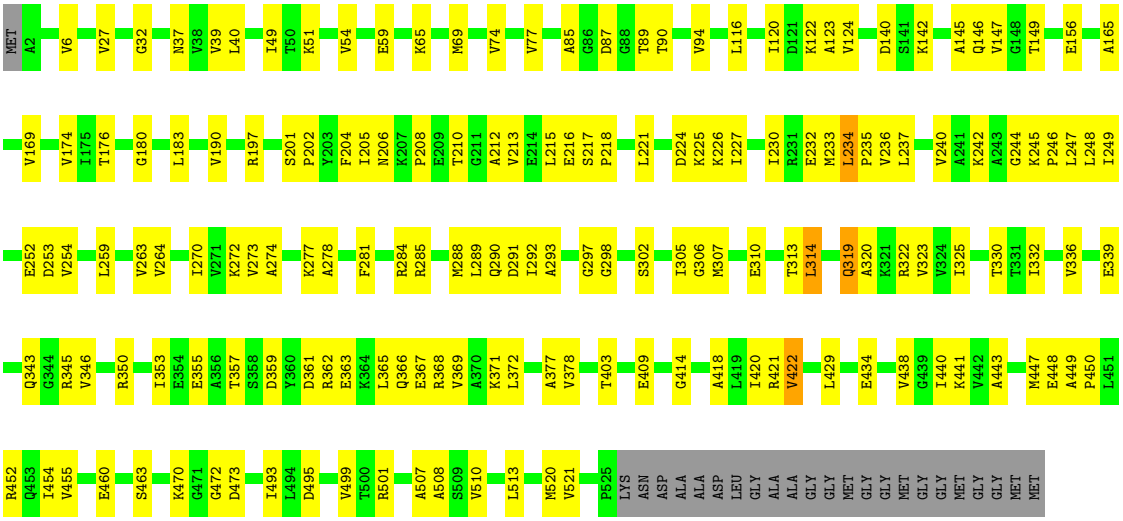
• Molecule 1: 60 kDa chaperonin

Chain D:



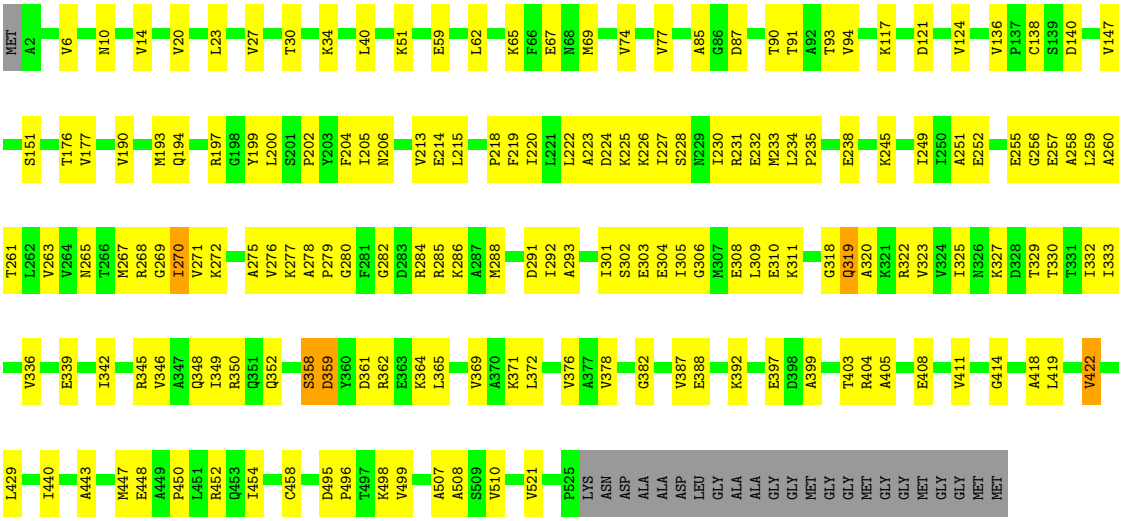
• Molecule 1: 60 kDa chaperonin

Chain K:



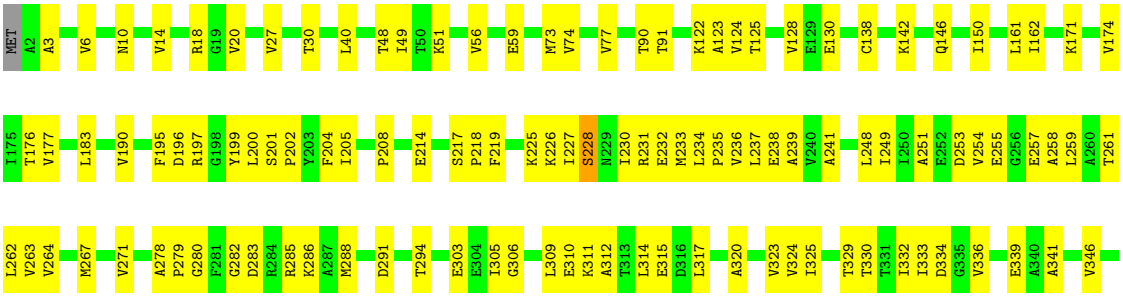
• Molecule 1: 60 kDa chaperonin

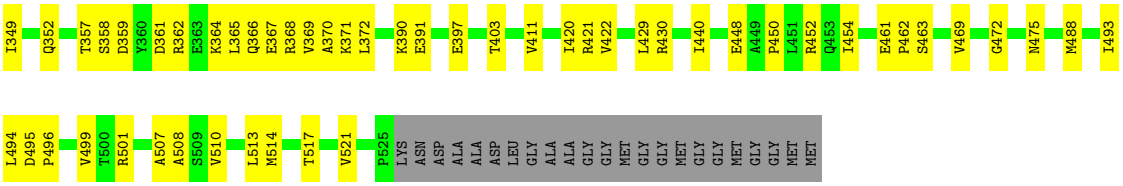
Chain J:



• Molecule 1: 60 kDa chaperonin

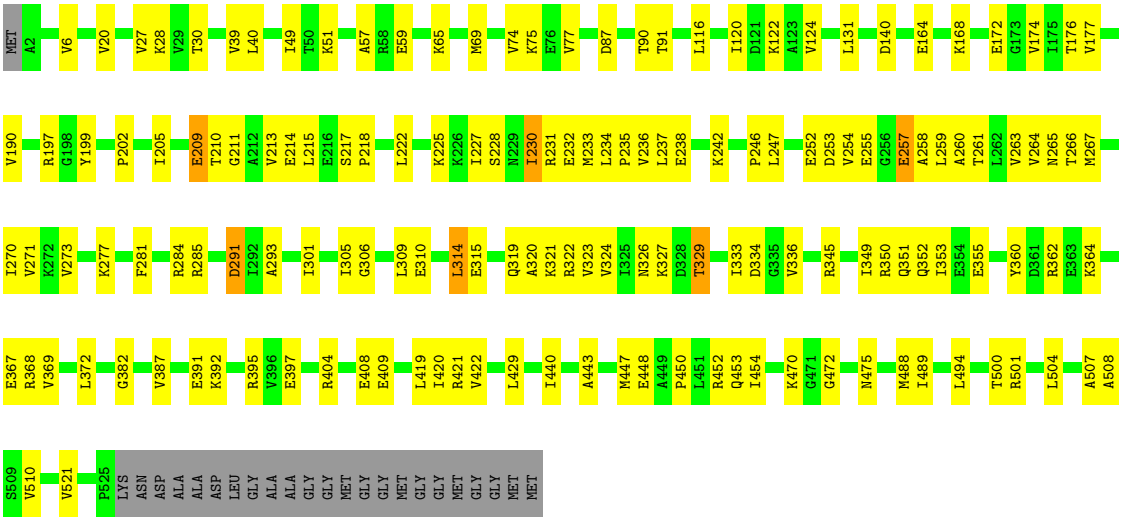
Chain I:





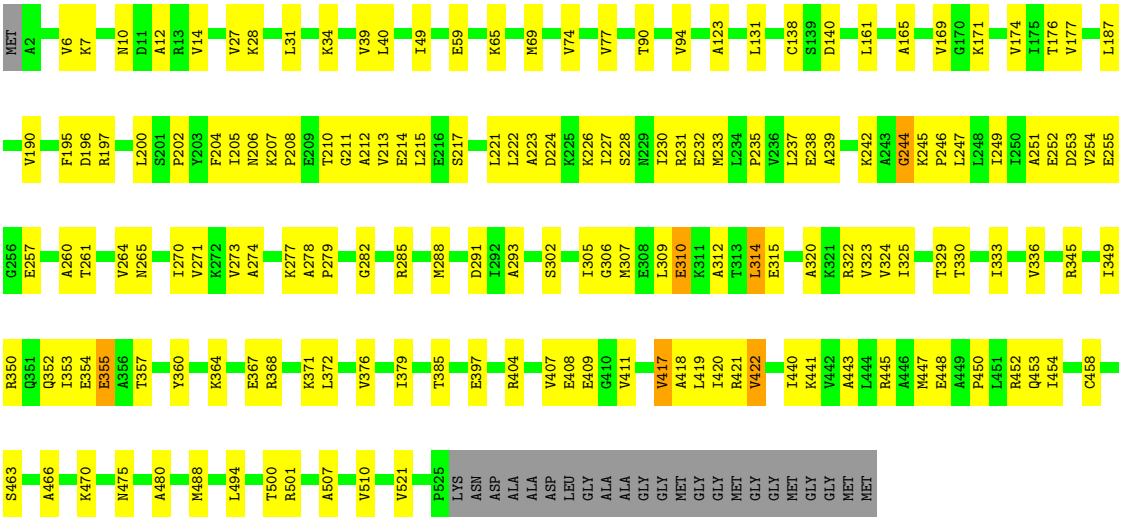
• Molecule 1: 60 kDa chaperonin

Chain L:



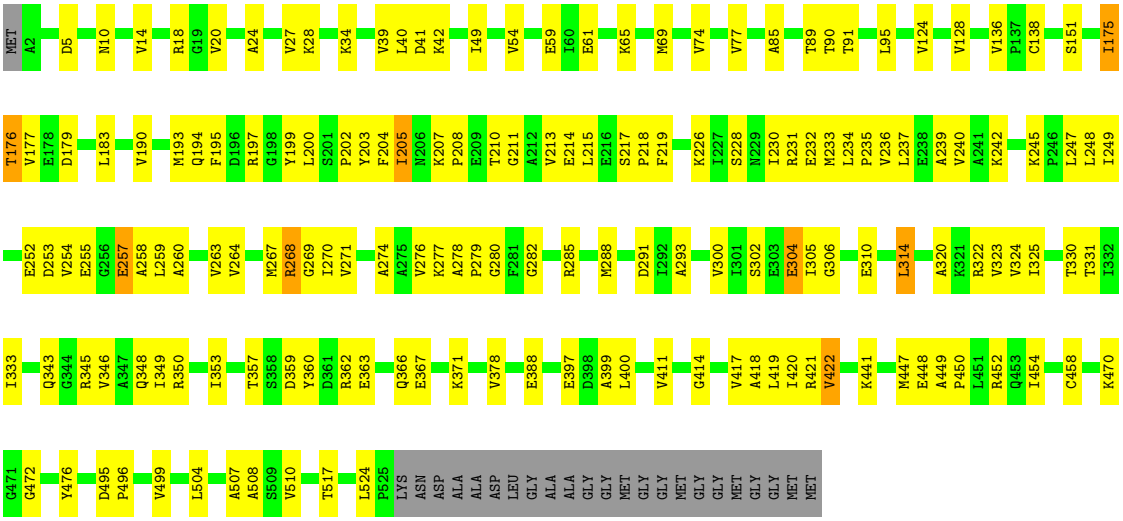
• Molecule 1: 60 kDa chaperonin

Chain M:



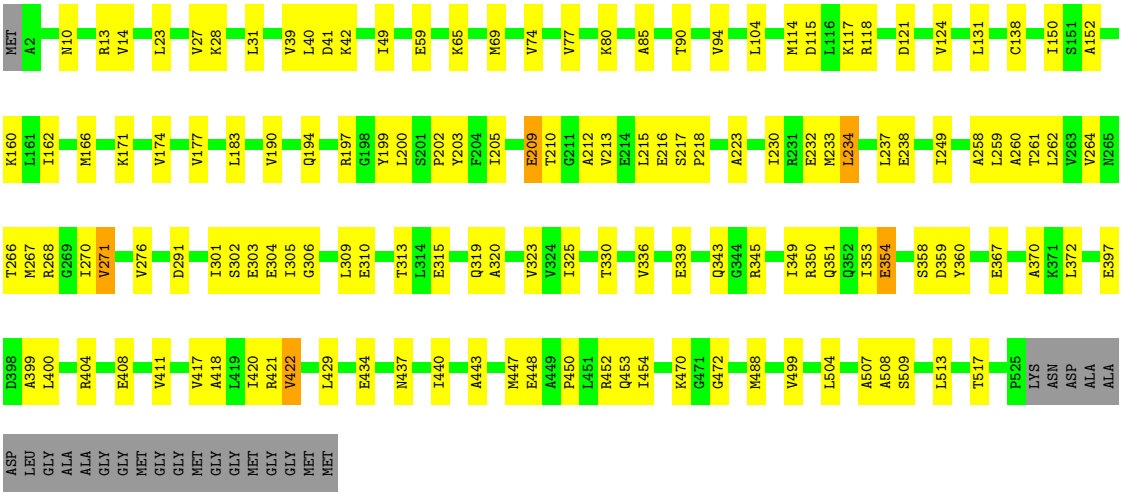
• Molecule 1: 60 kDa chaperonin

Chain H:



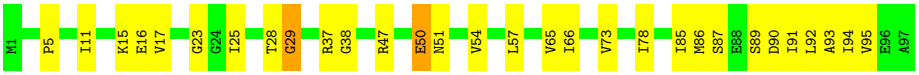
• Molecule 1: 60 kDa chaperonin

Chain N:



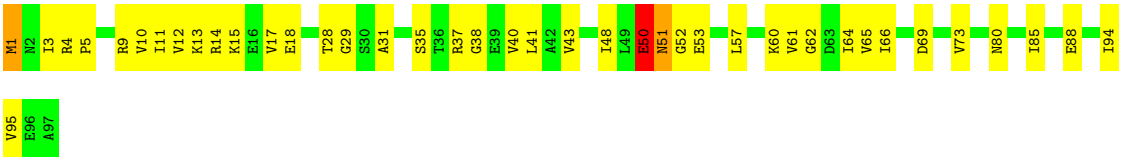
• Molecule 2: 10 kDa chaperonin

Chain O:



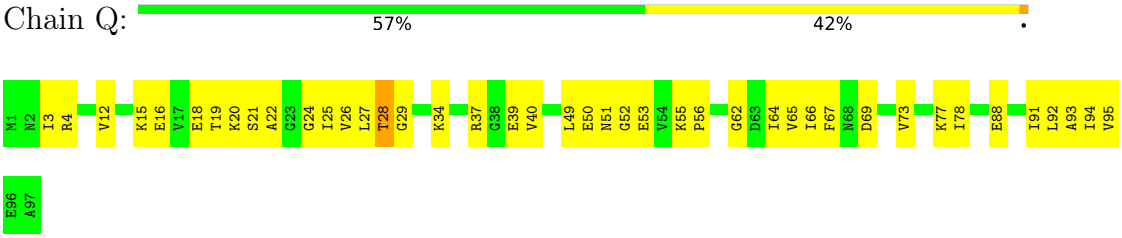
• Molecule 2: 10 kDa chaperonin

Chain P:



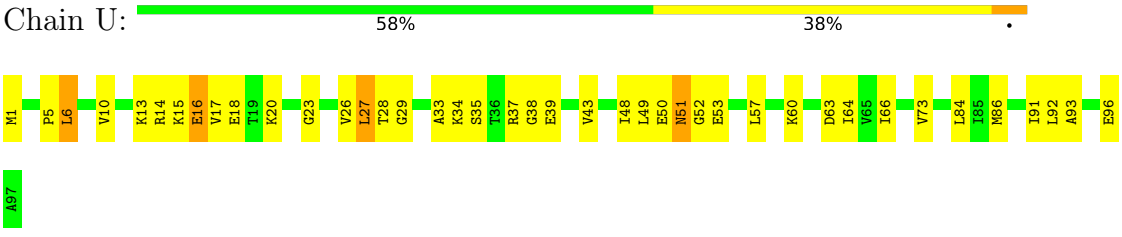
• Molecule 2: 10 kDa chaperonin

Chain Q:



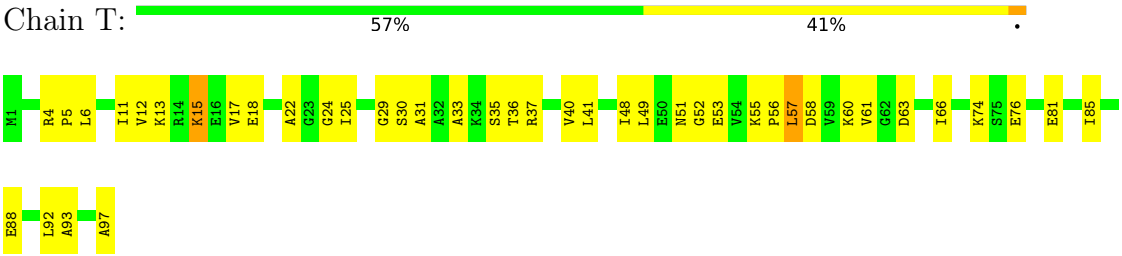
• Molecule 2: 10 kDa chaperonin

Chain U:



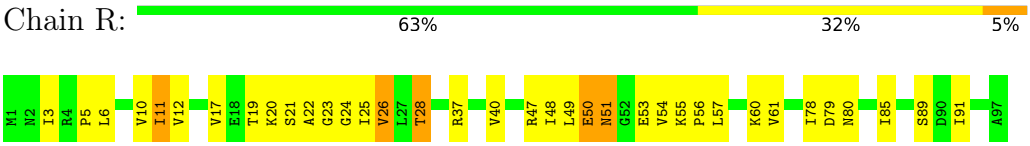
• Molecule 2: 10 kDa chaperonin

Chain T:



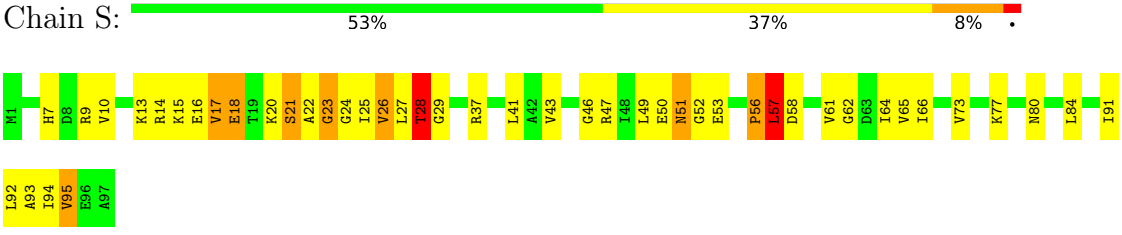
• Molecule 2: 10 kDa chaperonin

Chain R:



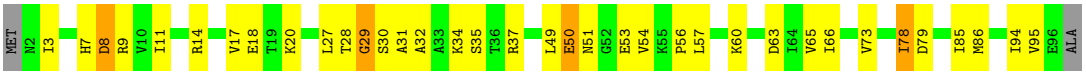
• Molecule 2: 10 kDa chaperonin

Chain S:



• Molecule 2: 10 kDa chaperonin

Chain X:



• Molecule 2: 10 kDa chaperonin

Chain W:

• Molecule 2: 10 kDa chaperonin

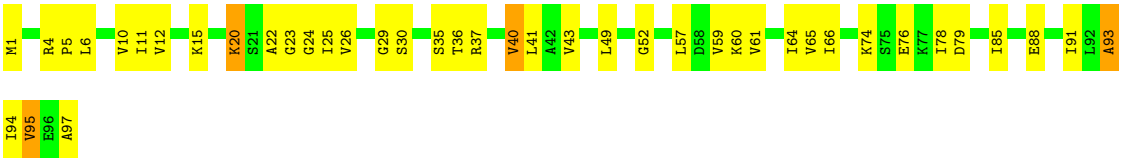
Chain V:

• Molecule 2: 10 kDa chaperonin

Chain Y:

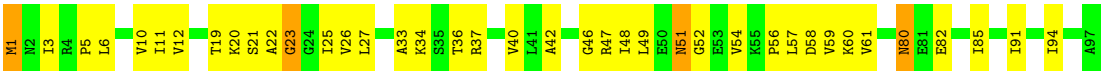
• Molecule 2: 10 kDa chaperonin

Chain Z:



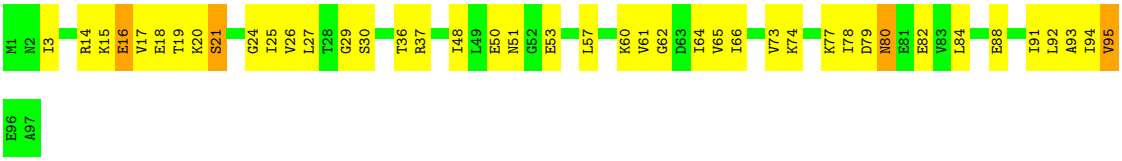
• Molecule 2: 10 kDa chaperonin

Chain 2:



• Molecule 2: 10 kDa chaperonin

Chain 1:


M1
N2
I3
R14
K15
E16
V17
E18
T19
K20
S21
G24
I25
V26
L27
T28
G29
S30
T36
R37
I48
L49
E50
N51
G52
E53
L57
K60
V61
G62
D63
I64
V65
I66
V73
K74
K77
I78
D79
N80
E81
E82
V83
L84
E88
I91
L92
A93
I94
V95
E96
A97

4 Data and refinement statistics (i)

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	171.95Å 173.65Å 411.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	122.19 – 3.66	Depositor
% Data completeness (in resolution range)	99.5 (122.19-3.66)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.34 (at 3.67Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.4_1496)	Depositor
R, R_{free}	0.188 , 0.241	Depositor
Wilson B-factor (Å^2)	87.5	Xtriage
Anisotropy	0.664	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	0.190 for k,h,-l	Xtriage
Total number of atoms	64579	wwPDB-VP
Average B, all atoms (Å^2)	106.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.93% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, K, BEF, 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	0.34	0/3883	0.56	0/5243
1	B	0.32	0/3883	0.55	0/5243
1	C	0.33	0/3883	0.58	0/5243
1	D	0.35	0/3883	0.60	1/5243 (0.0%)
1	E	0.33	0/3883	0.56	0/5243
1	F	0.33	0/3883	0.56	1/5243 (0.0%)
1	G	0.34	0/3883	0.57	1/5243 (0.0%)
1	H	0.32	0/3883	0.57	0/5243
1	I	0.32	0/3883	0.56	0/5243
1	J	0.33	0/3883	0.56	0/5243
1	K	0.33	0/3883	0.59	2/5243 (0.0%)
1	L	0.33	0/3883	0.55	1/5243 (0.0%)
1	M	0.33	0/3883	0.59	1/5243 (0.0%)
1	N	0.35	0/3883	0.59	1/5243 (0.0%)
2	1	0.33	0/731	0.64	0/983
2	2	0.33	0/731	0.72	2/983 (0.2%)
2	O	0.30	0/731	0.64	0/983
2	P	0.33	0/731	0.71	1/983 (0.1%)
2	Q	0.30	0/731	0.66	0/983
2	R	0.32	0/731	0.71	0/983
2	S	0.39	0/731	0.85	2/983 (0.2%)
2	T	0.30	0/731	0.65	1/983 (0.1%)
2	U	0.29	0/731	0.61	0/983
2	V	0.28	0/726	0.61	0/976
2	W	0.31	0/723	0.67	0/973
2	X	0.33	0/718	0.65	0/966
2	Y	0.29	0/726	0.66	0/976
2	Z	0.29	0/731	0.63	0/983
All	All	0.33	0/64565	0.59	14/87123 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if

the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	2
1	K	0	1
2	2	0	1
2	O	0	1
2	P	0	1
2	Q	0	1
2	S	0	4
2	T	0	1
2	W	0	1
2	X	0	1
2	Z	0	1
All	All	0	15

There are no bond length outliers.

The worst 5 of 14 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	52	GLY	N-CA-C	-6.49	96.87	113.10
1	M	244	GLY	N-CA-C	5.88	127.79	113.10
2	S	57	LEU	CA-CB-CG	-5.59	102.45	115.30
1	L	230	ILE	CG1-CB-CG2	-5.52	99.25	111.40
2	P	51	ASN	CA-C-N	5.51	127.23	116.20

There are no chirality outliers.

5 of 15 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	228	SER	Peptide
1	E	305	ILE	Peptide
2	O	29	GLY	Peptide
2	P	50	GLU	Peptide
2	Q	51	ASN	Peptide

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	3855	0	3974	109	0
1	B	3855	0	3976	117	0
1	C	3855	0	3975	125	0
1	D	3855	0	3976	101	0
1	E	3855	0	3976	131	0
1	F	3855	0	3975	99	0
1	G	3855	0	3975	113	0
1	H	3855	0	3976	125	0
1	I	3855	0	3975	124	0
1	J	3855	0	3975	133	0
1	K	3855	0	3974	124	0
1	L	3855	0	3975	107	0
1	M	3855	0	3975	128	0
1	N	3855	0	3976	90	0
2	1	727	0	762	43	0
2	2	727	0	762	41	0
2	O	727	0	762	23	0
2	P	727	0	762	41	0
2	Q	727	0	762	39	0
2	R	727	0	762	32	0
2	S	727	0	762	57	0
2	T	727	0	762	36	0
2	U	727	0	762	40	0
2	V	722	0	757	27	0
2	W	719	0	750	37	0
2	X	714	0	745	19	0
2	Y	722	0	757	28	0
2	Z	727	0	762	34	0
3	A	27	0	12	0	0
3	B	27	0	12	1	0
3	C	27	0	12	2	0
3	D	27	0	12	3	0
3	E	27	0	12	1	0
3	F	27	0	12	2	0
3	G	27	0	12	2	0
3	H	27	0	12	2	0
3	I	27	0	12	3	0
3	J	27	0	12	3	0
3	K	27	0	12	2	0
3	L	27	0	12	2	0
3	M	27	0	12	3	0
3	N	27	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	4	0	0	0	0
4	B	4	0	0	3	0
4	C	4	0	0	1	0
4	D	4	0	0	1	0
4	E	4	0	0	2	0
4	F	4	0	0	1	0
4	G	4	0	0	3	0
4	H	4	0	0	1	0
4	I	4	0	0	1	0
4	J	4	0	0	2	0
4	K	4	0	0	2	0
4	L	4	0	0	2	0
4	M	4	0	0	1	0
4	N	4	0	0	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	0	0
5	H	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
5	K	1	0	0	0	0
5	L	1	0	0	0	0
5	M	1	0	0	0	0
5	N	1	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
6	G	1	0	0	0	0
6	H	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	M	1	0	0	0	0
6	N	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	64579	0	66450	1996	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 15.

The worst 5 of 1996 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:226:LYS:HG2	1:C:252:GLU:HG2	1.39	1.03
1:C:239:ALA:HA	2:Q:25:ILE:HD11	1.43	1.01
1:E:238:GLU:HB2	2:S:22:ALA:HB1	1.45	0.97
2:S:28:THR:HG22	2:S:29:GLY:HA3	1.49	0.94
1:B:291:ASP:HB3	1:B:372:LEU:HD21	1.50	0.93

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	522/548 (95%)	506 (97%)	15 (3%)	1 (0%)	47	78
1	B	522/548 (95%)	502 (96%)	20 (4%)	0	100	100
1	C	522/548 (95%)	501 (96%)	20 (4%)	1 (0%)	47	78
1	D	522/548 (95%)	498 (95%)	23 (4%)	1 (0%)	47	78
1	E	522/548 (95%)	505 (97%)	16 (3%)	1 (0%)	47	78
1	F	522/548 (95%)	500 (96%)	21 (4%)	1 (0%)	47	78
1	G	522/548 (95%)	503 (96%)	18 (3%)	1 (0%)	47	78
1	H	522/548 (95%)	501 (96%)	21 (4%)	0	100	100
1	I	522/548 (95%)	503 (96%)	19 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	522/548 (95%)	500 (96%)	20 (4%)	2 (0%)	34 69
1	K	522/548 (95%)	505 (97%)	17 (3%)	0	100 100
1	L	522/548 (95%)	508 (97%)	14 (3%)	0	100 100
1	M	522/548 (95%)	502 (96%)	20 (4%)	0	100 100
1	N	522/548 (95%)	505 (97%)	17 (3%)	0	100 100
2	1	95/97 (98%)	83 (87%)	12 (13%)	0	100 100
2	2	95/97 (98%)	82 (86%)	12 (13%)	1 (1%)	14 51
2	O	95/97 (98%)	86 (90%)	8 (8%)	1 (1%)	14 51
2	P	95/97 (98%)	85 (90%)	10 (10%)	0	100 100
2	Q	95/97 (98%)	84 (88%)	11 (12%)	0	100 100
2	R	95/97 (98%)	85 (90%)	8 (8%)	2 (2%)	7 38
2	S	95/97 (98%)	77 (81%)	14 (15%)	4 (4%)	3 25
2	T	95/97 (98%)	87 (92%)	7 (7%)	1 (1%)	14 51
2	U	95/97 (98%)	84 (88%)	10 (10%)	1 (1%)	14 51
2	V	94/97 (97%)	84 (89%)	10 (11%)	0	100 100
2	W	94/97 (97%)	78 (83%)	15 (16%)	1 (1%)	14 51
2	X	93/97 (96%)	81 (87%)	10 (11%)	2 (2%)	6 37
2	Y	94/97 (97%)	86 (92%)	7 (7%)	1 (1%)	14 51
2	Z	95/97 (98%)	88 (93%)	7 (7%)	0	100 100
All	All	8633/9030 (96%)	8209 (95%)	402 (5%)	22 (0%)	41 74

5 of 22 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	270	ILE
1	E	305	ILE
1	C	230	ILE
1	D	230	ILE
2	S	26	VAL

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	404/415 (97%)	397 (98%)	7 (2%)	60	79
1	B	404/415 (97%)	397 (98%)	7 (2%)	60	79
1	C	404/415 (97%)	395 (98%)	9 (2%)	52	72
1	D	404/415 (97%)	396 (98%)	8 (2%)	55	74
1	E	404/415 (97%)	391 (97%)	13 (3%)	39	64
1	F	404/415 (97%)	397 (98%)	7 (2%)	60	79
1	G	404/415 (97%)	397 (98%)	7 (2%)	60	79
1	H	404/415 (97%)	391 (97%)	13 (3%)	39	64
1	I	404/415 (97%)	399 (99%)	5 (1%)	71	84
1	J	404/415 (97%)	397 (98%)	7 (2%)	60	79
1	K	404/415 (97%)	397 (98%)	7 (2%)	60	79
1	L	404/415 (97%)	394 (98%)	10 (2%)	47	69
1	M	404/415 (97%)	391 (97%)	13 (3%)	39	64
1	N	404/415 (97%)	394 (98%)	10 (2%)	47	69
2	1	80/80 (100%)	75 (94%)	5 (6%)	18	49
2	2	80/80 (100%)	76 (95%)	4 (5%)	24	55
2	O	80/80 (100%)	79 (99%)	1 (1%)	69	82
2	P	80/80 (100%)	78 (98%)	2 (2%)	47	69
2	Q	80/80 (100%)	79 (99%)	1 (1%)	69	82
2	R	80/80 (100%)	76 (95%)	4 (5%)	24	55
2	S	80/80 (100%)	75 (94%)	5 (6%)	18	49
2	T	80/80 (100%)	79 (99%)	1 (1%)	69	82
2	U	80/80 (100%)	76 (95%)	4 (5%)	24	55
2	V	80/80 (100%)	79 (99%)	1 (1%)	69	82
2	W	79/80 (99%)	78 (99%)	1 (1%)	69	82
2	X	79/80 (99%)	75 (95%)	4 (5%)	24	55
2	Y	80/80 (100%)	80 (100%)	0	100	100
2	Z	80/80 (100%)	76 (95%)	4 (5%)	24	55
All	All	6774/6930 (98%)	6614 (98%)	160 (2%)	49	70

5 of 160 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	360	TYR
2	X	53	GLU
1	H	136	VAL
1	H	422	VAL
2	Z	95	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	206	ASN
2	T	51	ASN
1	M	505	GLN
1	J	206	ASN
1	F	194	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 56 ligands modelled in this entry, 28 are monoatomic - leaving 28 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	$\#\|Z\|>2$
4	BEF	G	602	-	0,3,3	-	-	-		
4	BEF	J	602	-	0,3,3	-	-	-		
3	ADP	H	601	6,5	24,29,29	0.99	1 (4%)	29,45,45	1.40	4 (13%)
3	ADP	F	601	6,5	24,29,29	0.93	1 (4%)	29,45,45	1.56	5 (17%)
4	BEF	F	602	-	0,3,3	-	-	-		
3	ADP	M	601	6,5	24,29,29	0.98	1 (4%)	29,45,45	1.31	2 (6%)
3	ADP	E	601	6,5	24,29,29	1.02	1 (4%)	29,45,45	1.34	3 (10%)
4	BEF	L	602	-	0,3,3	-	-	-		
3	ADP	D	601	6,5	24,29,29	0.98	1 (4%)	29,45,45	1.42	3 (10%)
3	ADP	J	601	6,5	24,29,29	0.94	1 (4%)	29,45,45	1.33	3 (10%)
3	ADP	A	601	6,5	24,29,29	0.96	1 (4%)	29,45,45	1.48	4 (13%)
4	BEF	K	602	-	0,3,3	-	-	-		
4	BEF	B	602	-	0,3,3	-	-	-		
3	ADP	G	601	6,5	24,29,29	0.95	1 (4%)	29,45,45	1.40	3 (10%)
4	BEF	I	602	-	0,3,3	-	-	-		
4	BEF	C	602	-	0,3,3	-	-	-		
3	ADP	L	601	6,5	24,29,29	0.99	1 (4%)	29,45,45	1.48	4 (13%)
3	ADP	N	601	6,5	24,29,29	1.00	2 (8%)	29,45,45	1.47	3 (10%)
4	BEF	H	602	-	0,3,3	-	-	-		
3	ADP	K	601	6,5	24,29,29	0.98	1 (4%)	29,45,45	1.41	3 (10%)
3	ADP	C	601	6,5	24,29,29	0.96	1 (4%)	29,45,45	1.33	3 (10%)
3	ADP	B	601	6,5	24,29,29	0.92	1 (4%)	29,45,45	1.44	5 (17%)
4	BEF	E	602	-	0,3,3	-	-	-		
4	BEF	D	602	-	0,3,3	-	-	-		
3	ADP	I	601	6,5	24,29,29	0.95	1 (4%)	29,45,45	1.42	4 (13%)
4	BEF	N	602	-	0,3,3	-	-	-		
4	BEF	A	602	-	0,3,3	-	-	-		
4	BEF	M	602	-	0,3,3	-	-	-		

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
3	ADP	E	601	6,5	-	4/12/32/32	0/3/3/3
3	ADP	K	601	6,5	-	3/12/32/32	0/3/3/3
3	ADP	D	601	6,5	-	3/12/32/32	0/3/3/3
3	ADP	C	601	6,5	-	3/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	ADP	J	601	6,5	-	7/12/32/32	0/3/3/3
3	ADP	B	601	6,5	-	5/12/32/32	0/3/3/3
3	ADP	A	601	6,5	-	5/12/32/32	0/3/3/3
3	ADP	H	601	6,5	-	5/12/32/32	0/3/3/3
3	ADP	F	601	6,5	-	4/12/32/32	0/3/3/3
3	ADP	I	601	6,5	-	4/12/32/32	0/3/3/3
3	ADP	L	601	6,5	-	4/12/32/32	0/3/3/3
3	ADP	G	601	6,5	-	5/12/32/32	0/3/3/3
3	ADP	M	601	6,5	-	8/12/32/32	0/3/3/3
3	ADP	N	601	6,5	-	4/12/32/32	0/3/3/3

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	M	601	ADP	C5-C4	2.46	1.47	1.40
3	D	601	ADP	C5-C4	2.45	1.47	1.40
3	L	601	ADP	C5-C4	2.40	1.47	1.40
3	C	601	ADP	C5-C4	2.40	1.47	1.40
3	K	601	ADP	C5-C4	2.36	1.47	1.40

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	601	ADP	PA-O3A-PB	-4.18	118.48	132.83
3	N	601	ADP	PA-O3A-PB	-3.89	119.49	132.83
3	H	601	ADP	PA-O3A-PB	-3.64	120.35	132.83
3	A	601	ADP	PA-O3A-PB	-3.58	120.54	132.83
3	K	601	ADP	PA-O3A-PB	-3.53	120.72	132.83

There are no chirality outliers.

5 of 64 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	601	ADP	C5'-O5'-PA-O1A
3	F	601	ADP	O4'-C4'-C5'-O5'
3	F	601	ADP	C3'-C4'-C5'-O5'
3	E	601	ADP	PA-O3A-PB-O3B
3	E	601	ADP	C5'-O5'-PA-O1A

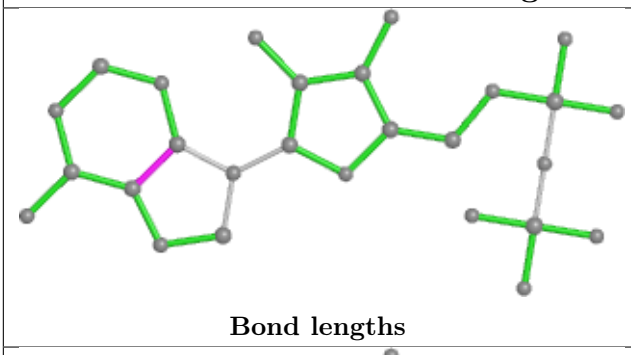
There are no ring outliers.

26 monomers are involved in 34 short contacts:

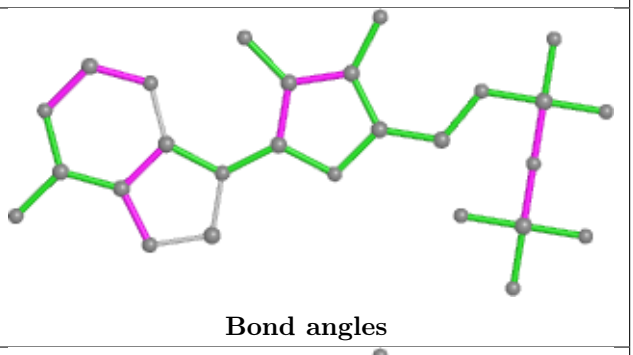
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	G	602	BEF	3	0
4	J	602	BEF	2	0
3	H	601	ADP	2	0
3	F	601	ADP	2	0
4	F	602	BEF	1	0
3	M	601	ADP	3	0
3	E	601	ADP	1	0
4	L	602	BEF	2	0
3	D	601	ADP	3	0
3	J	601	ADP	3	0
4	K	602	BEF	2	0
4	B	602	BEF	3	0
3	G	601	ADP	2	0
4	I	602	BEF	1	0
4	C	602	BEF	1	0
3	L	601	ADP	2	0
3	N	601	ADP	1	0
4	H	602	BEF	1	0
3	K	601	ADP	2	0
3	C	601	ADP	2	0
3	B	601	ADP	1	0
4	E	602	BEF	2	0
4	D	602	BEF	1	0
3	I	601	ADP	3	0
4	N	602	BEF	1	0
4	M	602	BEF	1	0

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

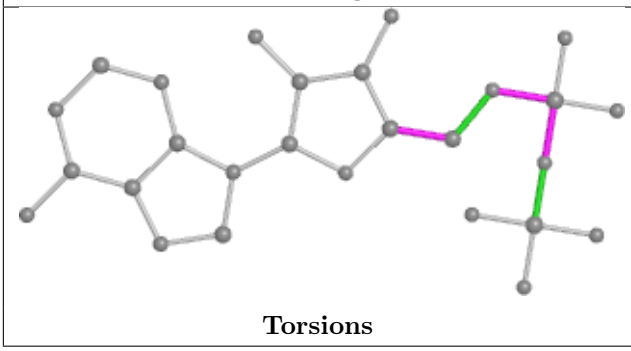
Ligand ADP H 601



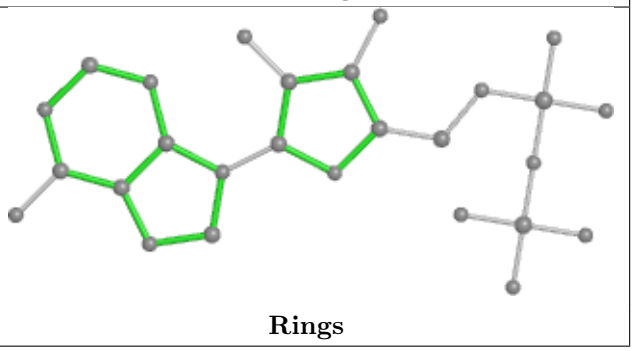
Bond lengths



Bond angles

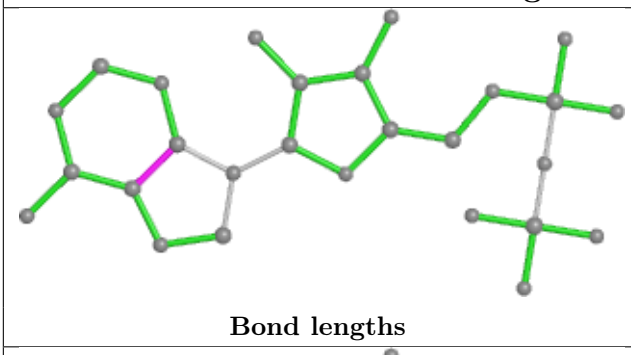


Torsions



Rings

Ligand ADP F 601



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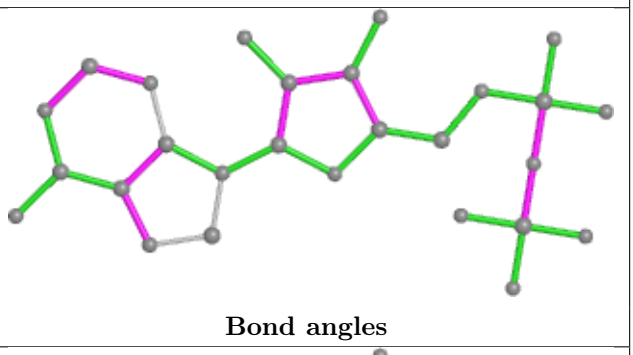

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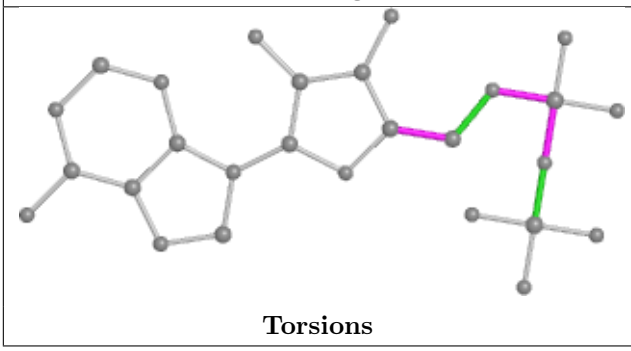

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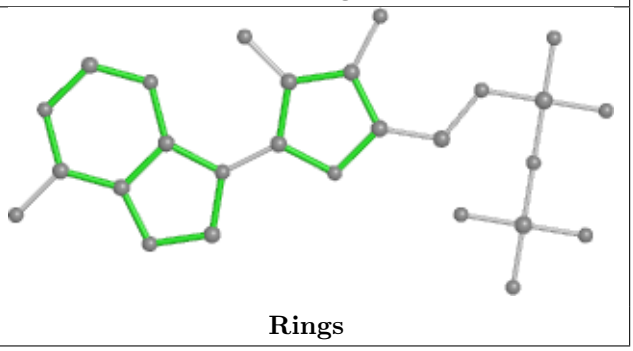

Rings

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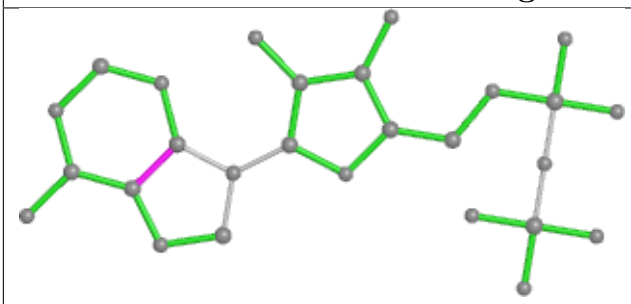

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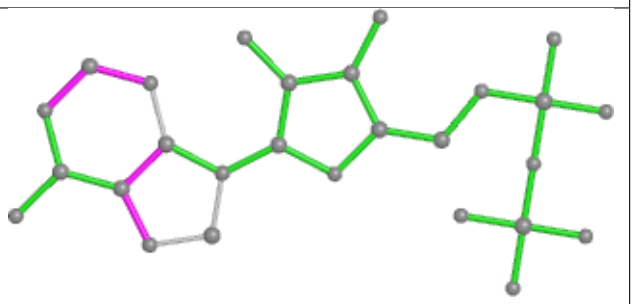
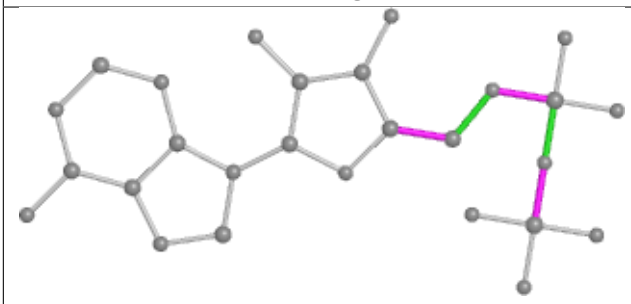


Bond angles



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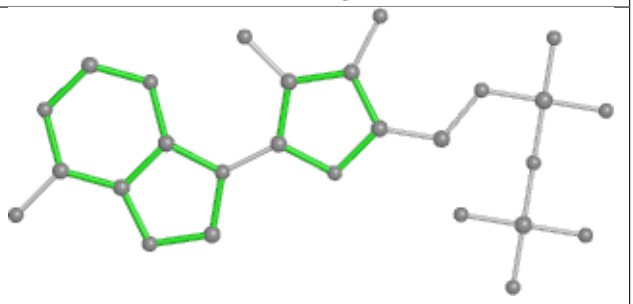
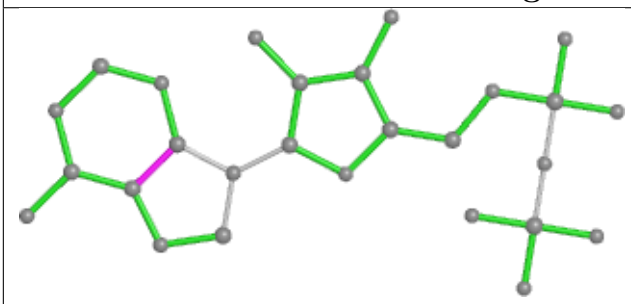


Rings

Ligand ADP E 601



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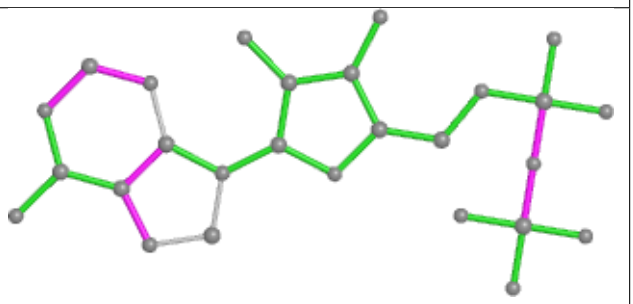

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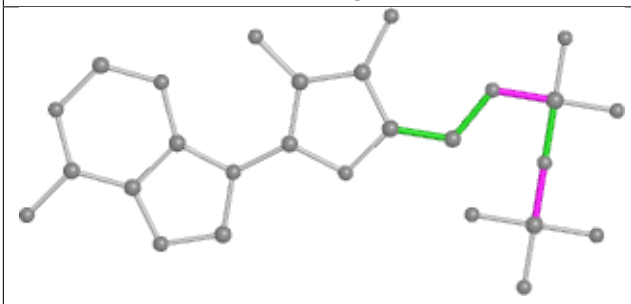

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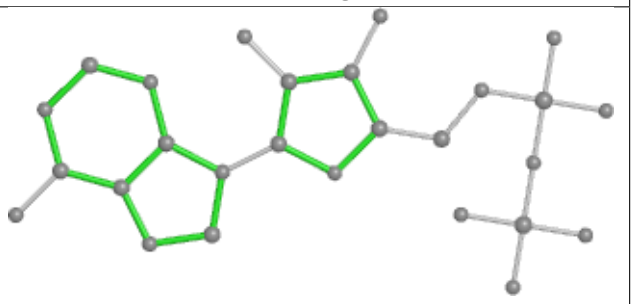
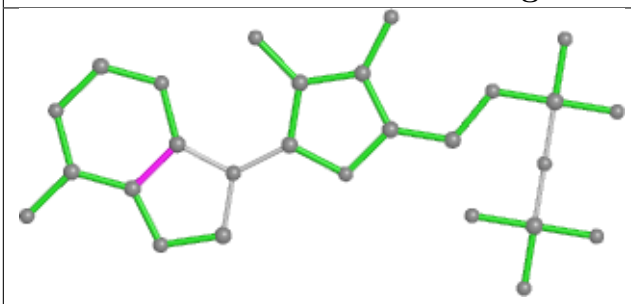


Rings

Ligand ADP D 601



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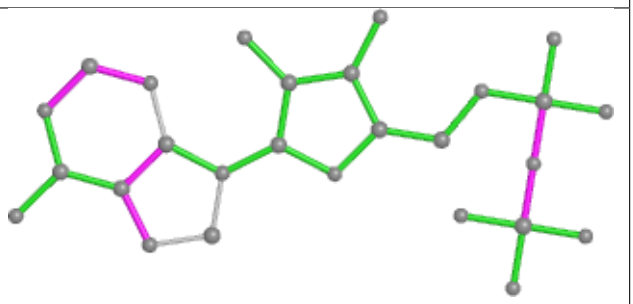

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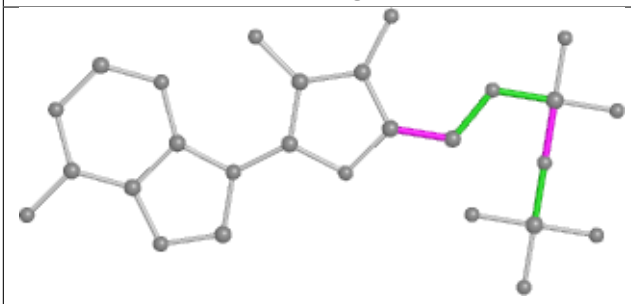

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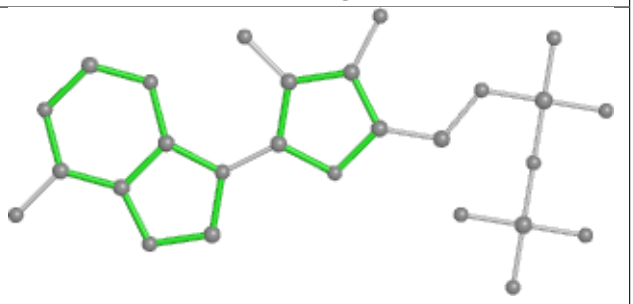

Rings

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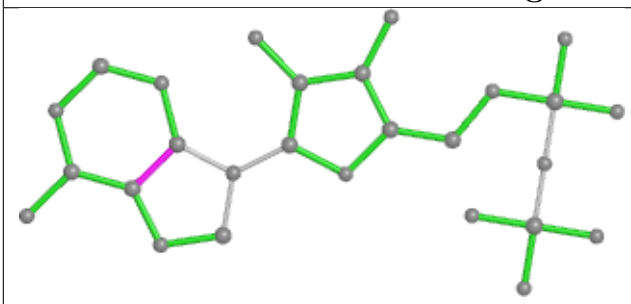

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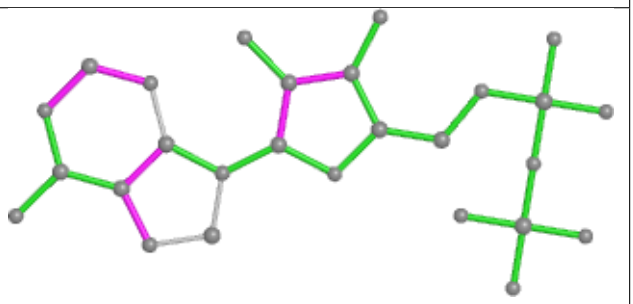

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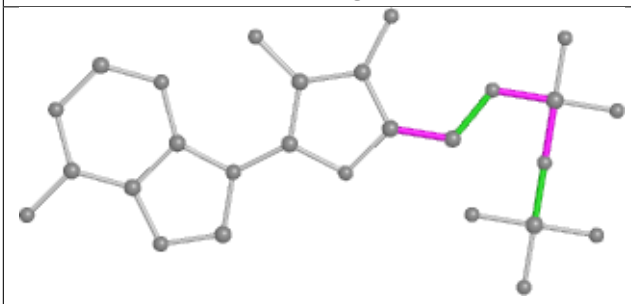

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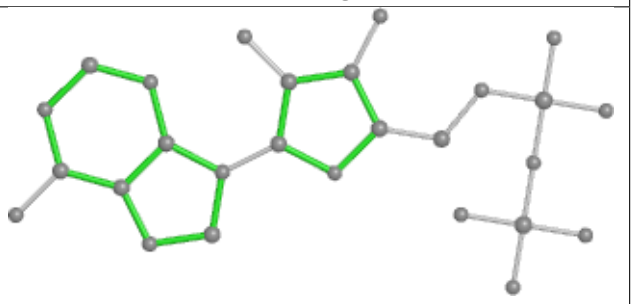

Rings

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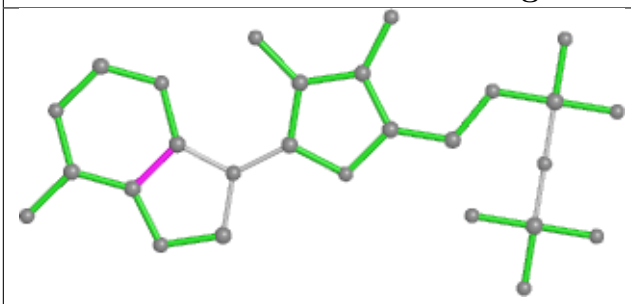

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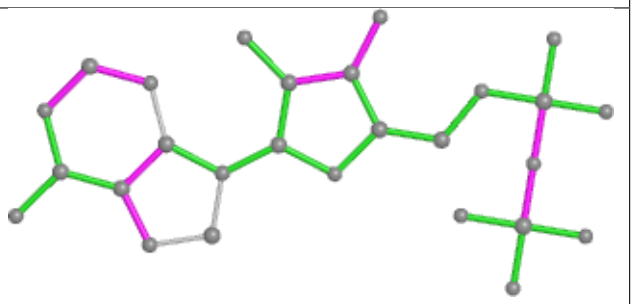

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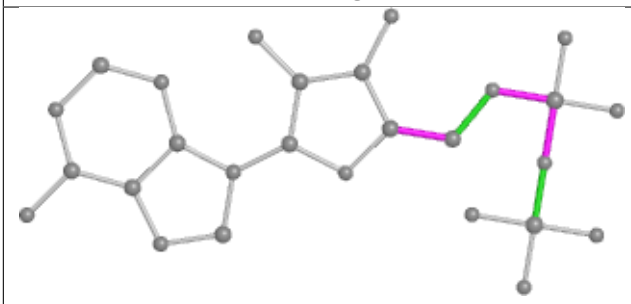

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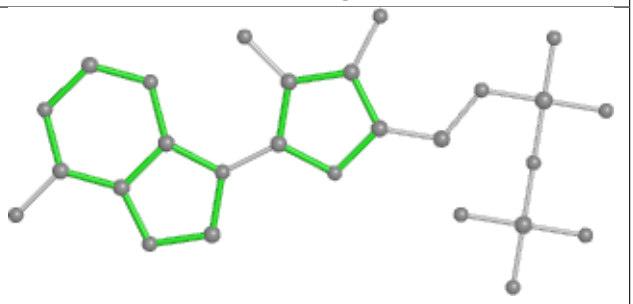

Rings

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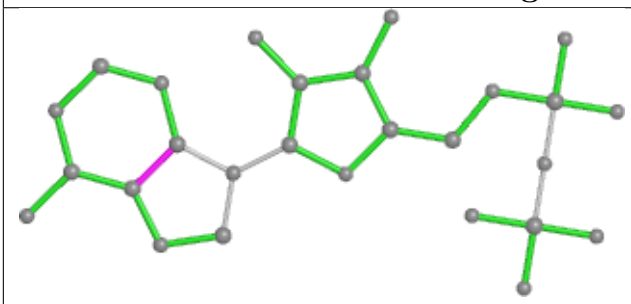

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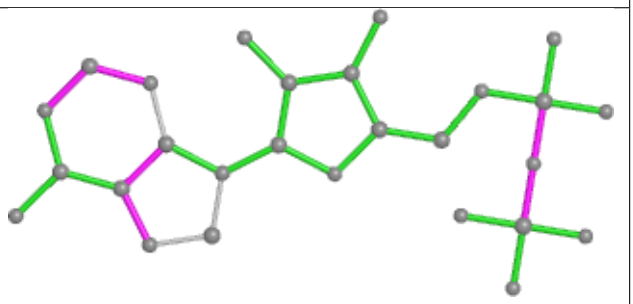

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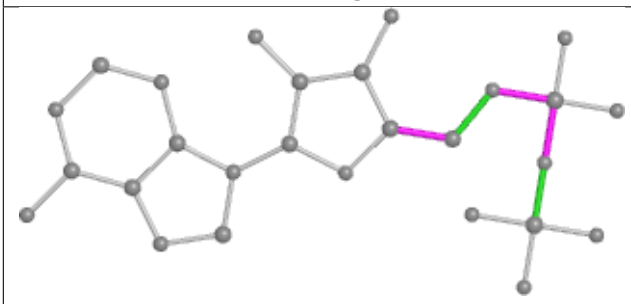

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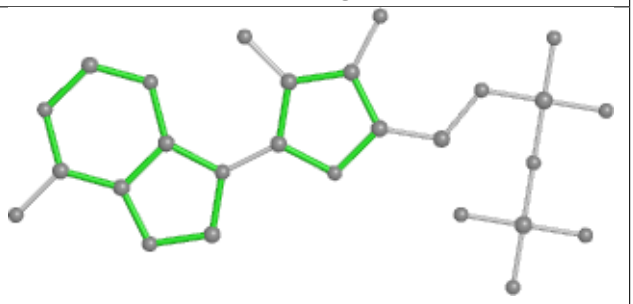
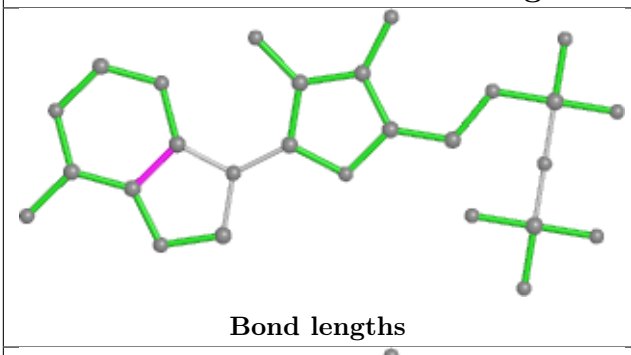


Rings

Ligand ADP L 601



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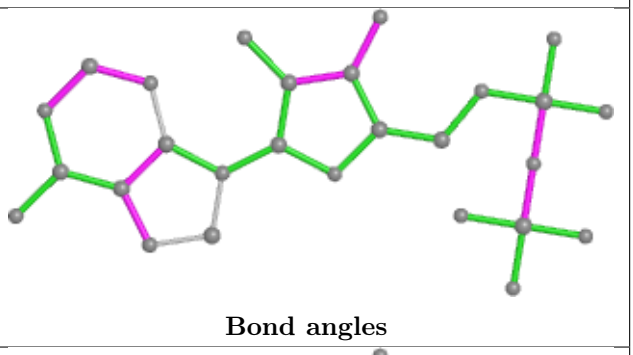

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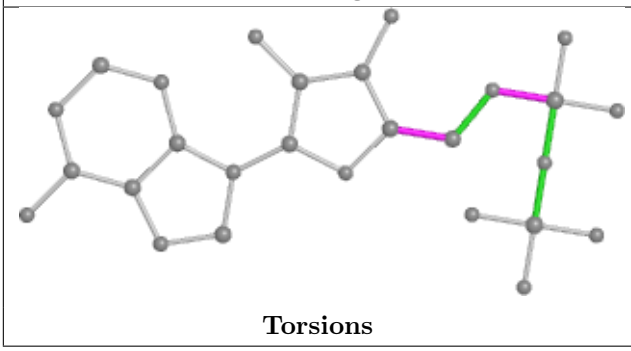

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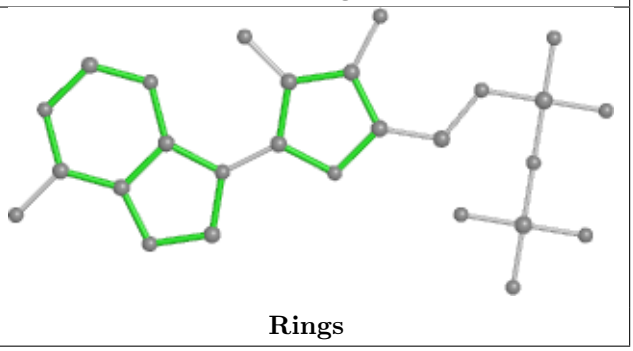
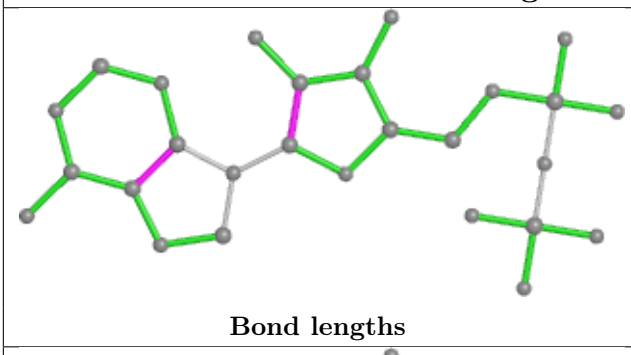


Rings

Ligand ADP N 601



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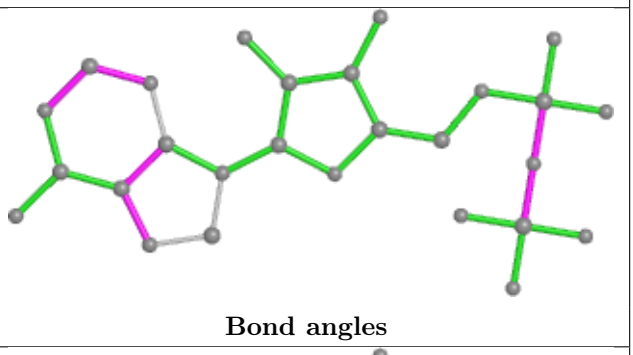

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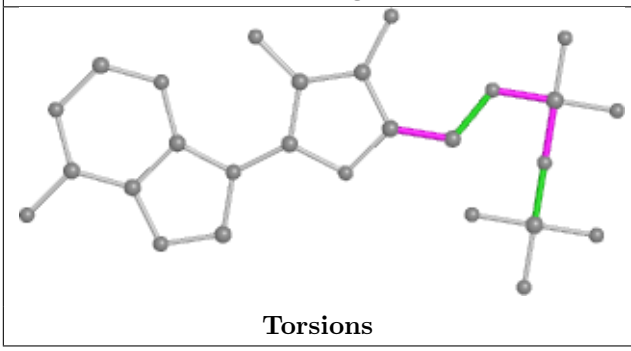

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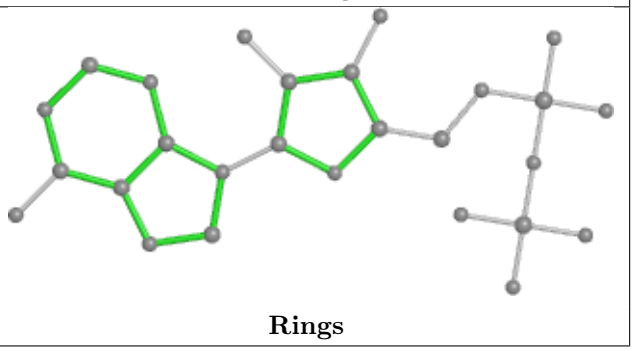
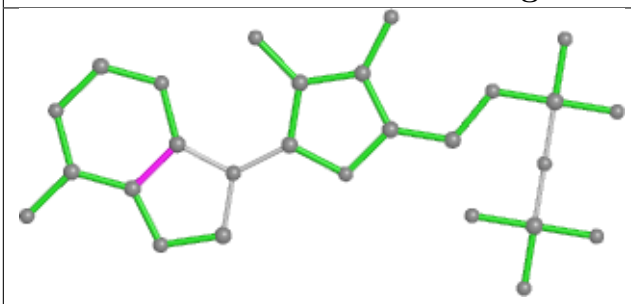


Rings

Ligand ADP K 601



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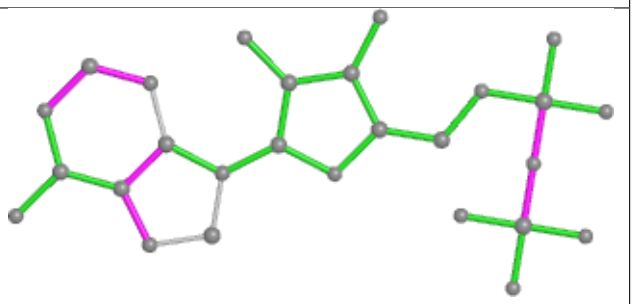

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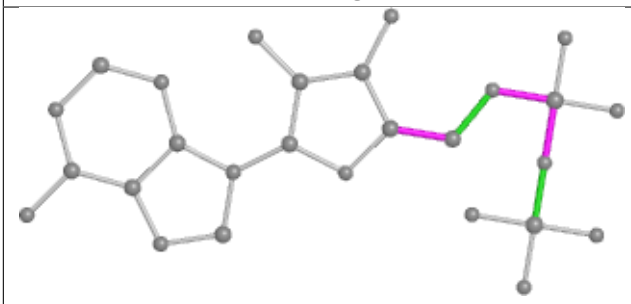

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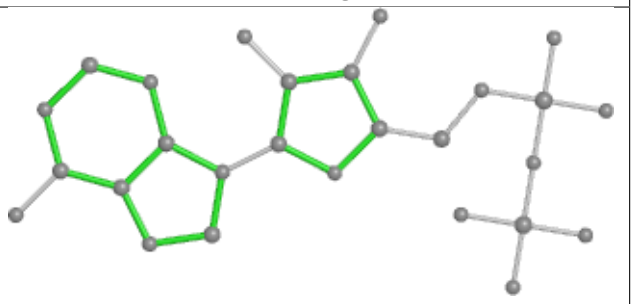
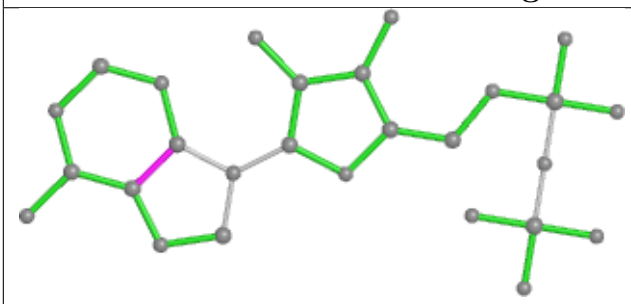
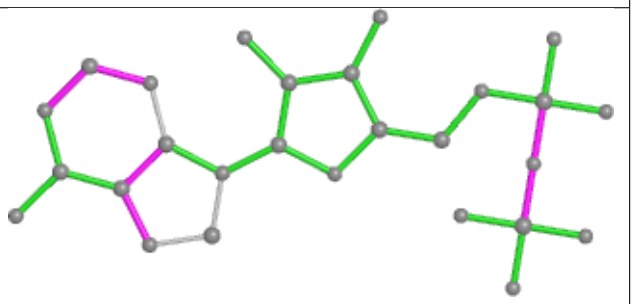


Rings

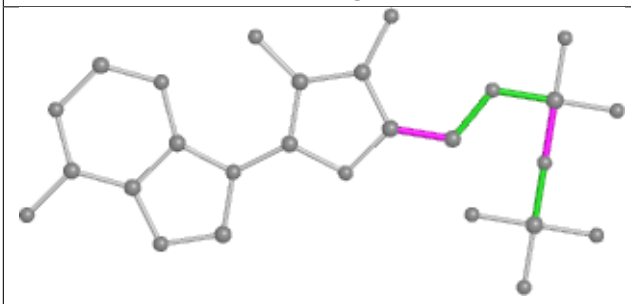
Ligand ADP C 601



Bond lengths



Bond angles



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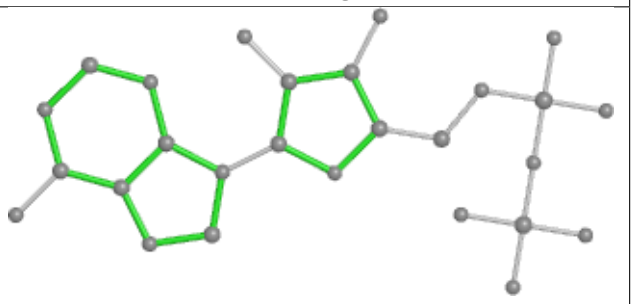
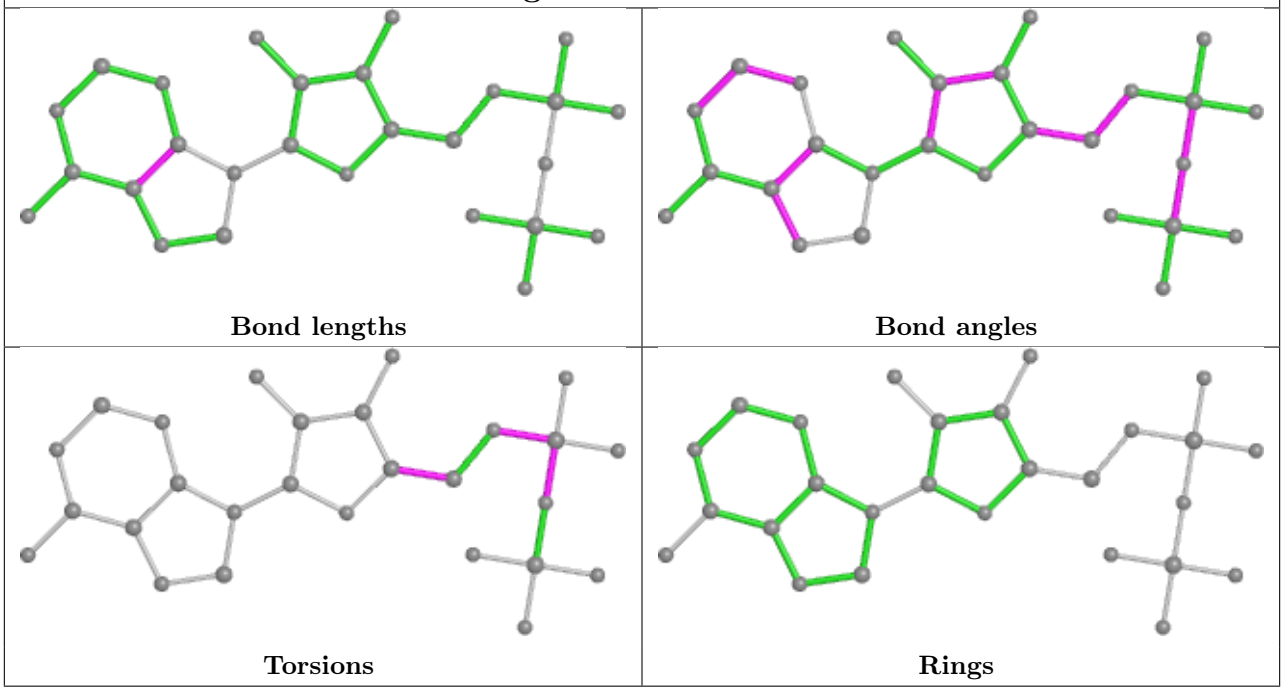
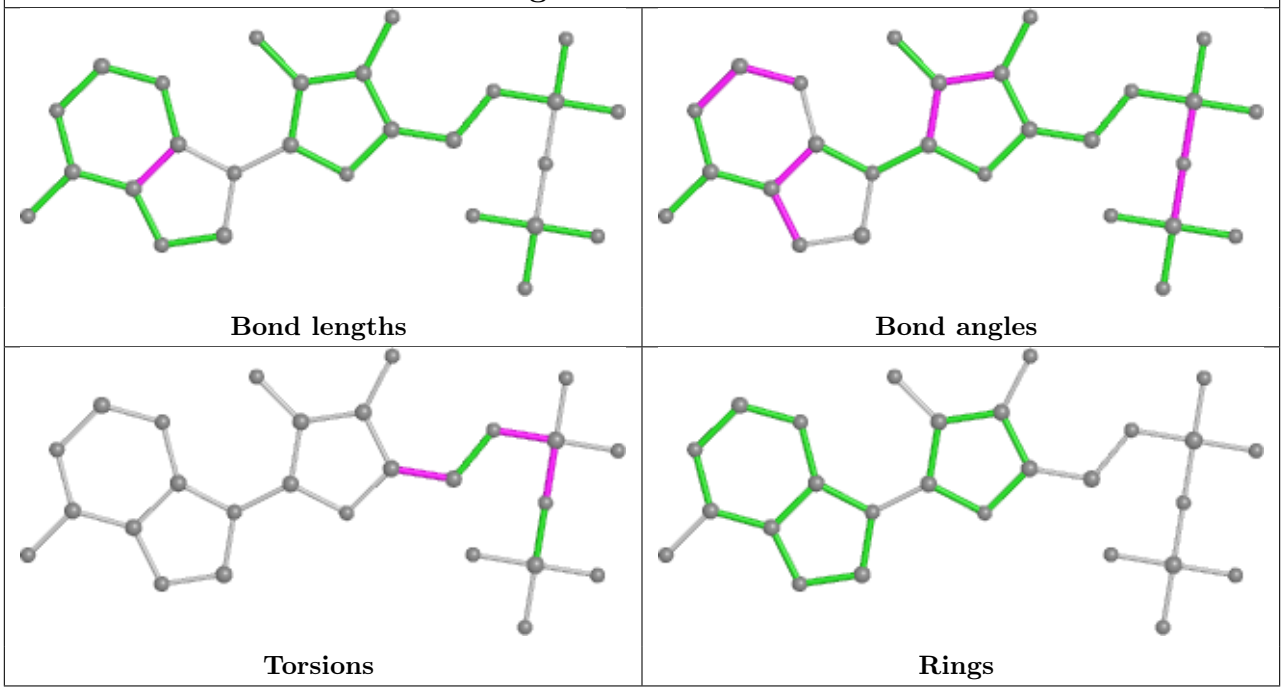


Rings

Ligand ADP B 601



Ligand ADP I 601



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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

6.3 Carbohydrates

EDS failed to run properly - this section is therefore empty.

6.4 Ligands

EDS failed to run properly - this section is therefore empty.

6.5 Other polymers

EDS failed to run properly - this section is therefore empty.