



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 12, 2026 – 02:30 PM UTC

PDB ID : 4V4O / pdb_00004v4o
Title : Crystal Structure of the Chaperonin Complex Cpn60/Cpn10/(ADP)7 from Thermus Thermophilus
Authors : Shimamura, T.; Koike-Takeshita, A.; Yokoyama, K.; Masui, R.; Murai, N.; Yoshida, M.; Taguchi, H.; Iwata, S.
Deposited on : 2004-05-23
Resolution : 2.80 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 ⓘ 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 ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

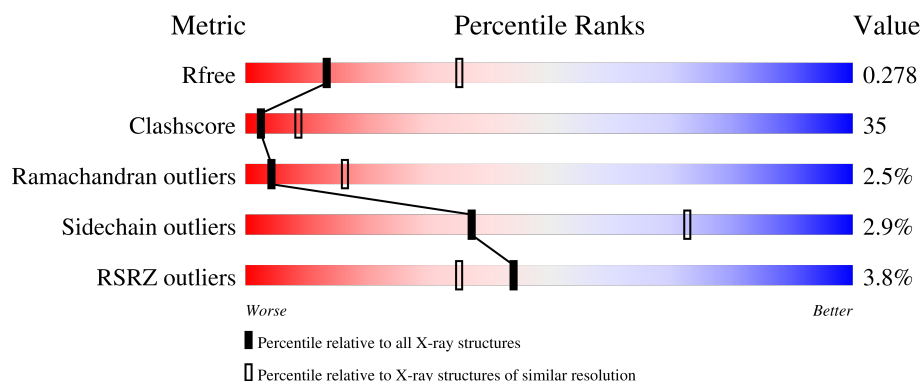
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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 $\leq 5\%$. 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	543	
1	B	543	
1	C	543	
1	D	543	

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Mol	Chain	Length	Quality of chain
1	E	543	
1	F	543	
1	G	543	
1	H	543	
1	I	543	
1	J	543	
1	K	543	
1	L	543	
1	M	543	
1	N	543	
1	a	543	
1	b	543	
1	c	543	
1	d	543	
1	e	543	
1	f	543	
1	g	543	
1	h	543	
1	i	543	
1	j	543	
1	k	543	
1	l	543	
1	m	543	
1	n	543	
2	O	100	

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Mol	Chain	Length	Quality of chain
2	P	100	
2	Q	100	
2	R	100	
2	S	100	
2	T	100	
2	U	100	
2	o	100	
2	p	100	
2	q	100	
2	r	100	
2	s	100	
2	t	100	
2	u	100	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 121267 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 cpn60(GroEL).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	B	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	C	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	D	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	E	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	F	529	Total	C	N	O	S	0	0	0
			3974	2495	689	785	5			
1	G	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	H	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	I	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	J	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	K	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	L	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	M	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	N	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	a	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	b	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	c	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	d	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	e	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	f	527	Total	C	N	O	S	0	0	0
			3956	2484	686	781	5			
1	g	526	Total	C	N	O	S	0	0	0
			3947	2478	684	780	5			
1	h	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	i	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	j	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	k	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	l	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	m	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			
1	n	525	Total	C	N	O	S	0	0	0
			3938	2473	683	777	5			

- Molecule 2 is a protein called cpn10(GroES).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	96	Total	C	N	O		0	0	0
			739	470	126	143				
2	P	94	Total	C	N	O		0	0	0
			723	460	123	140				
2	Q	96	Total	C	N	O		0	0	0
			739	470	126	143				
2	R	96	Total	C	N	O		0	0	0
			739	470	126	143				
2	S	96	Total	C	N	O		0	0	0
			739	470	126	143				
2	T	96	Total	C	N	O		0	0	0
			739	470	126	143				
2	U	96	Total	C	N	O		0	0	0
			739	470	126	143				

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	o	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	p	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	q	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	r	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	s	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	t	96	Total	C	N	O	0	0	0
			739	470	126	143			
2	u	96	Total	C	N	O	0	0	0
			739	470	126	143			

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

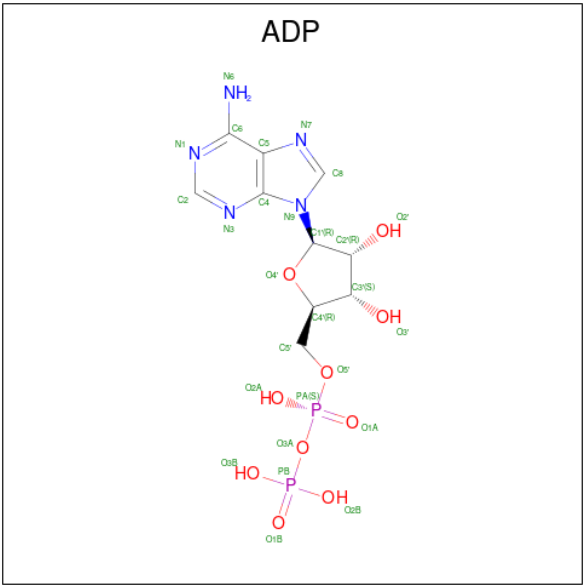
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mg	0	0
			1	1		
3	B	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	E	1	Total	Mg	0	0
			1	1		
3	F	1	Total	Mg	0	0
			1	1		
3	G	1	Total	Mg	0	0
			1	1		
3	a	1	Total	Mg	0	0
			1	1		
3	b	1	Total	Mg	0	0
			1	1		
3	c	1	Total	Mg	0	0
			1	1		
3	d	1	Total	Mg	0	0
			1	1		
3	e	1	Total	Mg	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	f	1	Total	Mg	0	0
			1	1		
3	g	1	Total	Mg	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



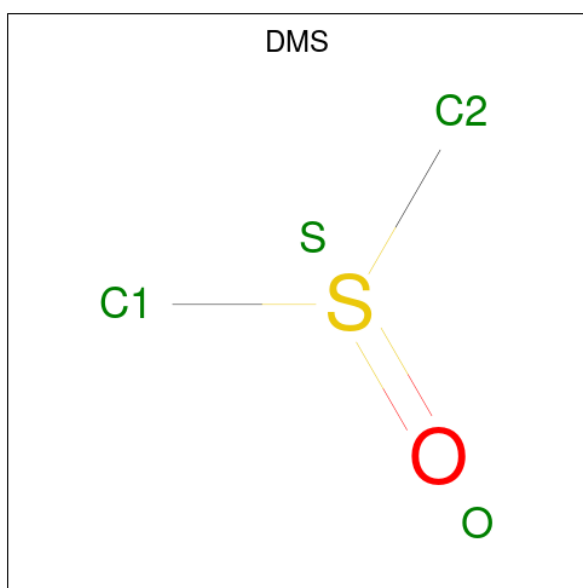
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	G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

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	c	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	d	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	e	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	f	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	g	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C₂H₆OS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	H	1	Total	C	O	S	0	0
			4	2	1	1		
5	I	1	Total	C	O	S	0	0
			4	2	1	1		
5	J	1	Total	C	O	S	0	0
			4	2	1	1		
5	K	1	Total	C	O	S	0	0
			4	2	1	1		
5	L	1	Total	C	O	S	0	0
			4	2	1	1		
5	M	1	Total	C	O	S	0	0
			4	2	1	1		

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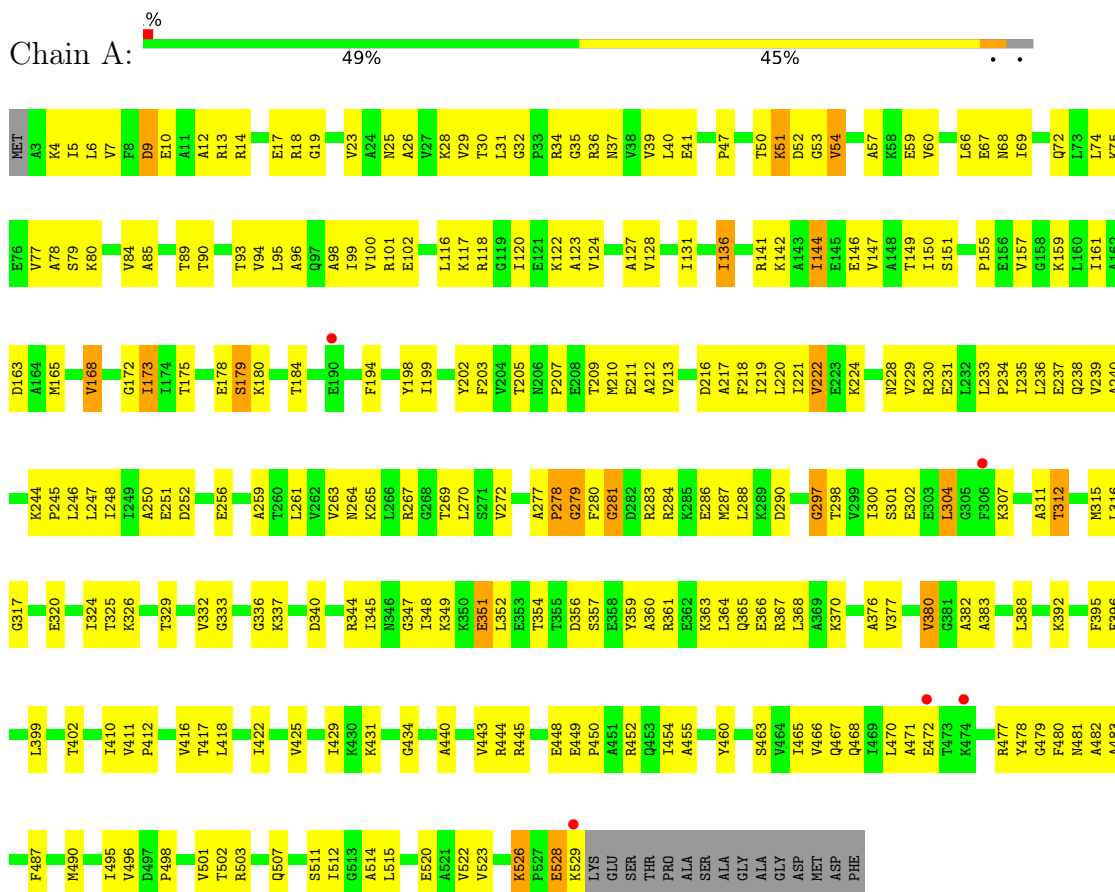
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	N	1	Total 4	C 2	O 1	S 1	0	0
5	h	1	Total 4	C 2	O 1	S 1	0	0
5	i	1	Total 4	C 2	O 1	S 1	0	0
5	j	1	Total 4	C 2	O 1	S 1	0	0
5	k	1	Total 4	C 2	O 1	S 1	0	0
5	l	1	Total 4	C 2	O 1	S 1	0	0
5	m	1	Total 4	C 2	O 1	S 1	0	0
5	n	1	Total 4	C 2	O 1	S 1	0	0

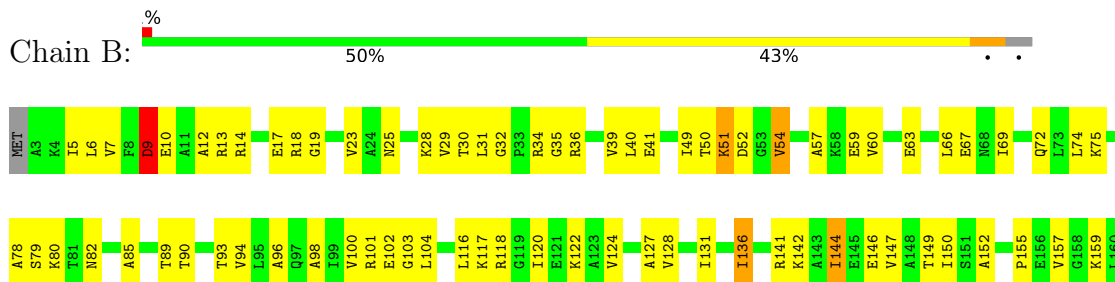
3 Residue-property plots

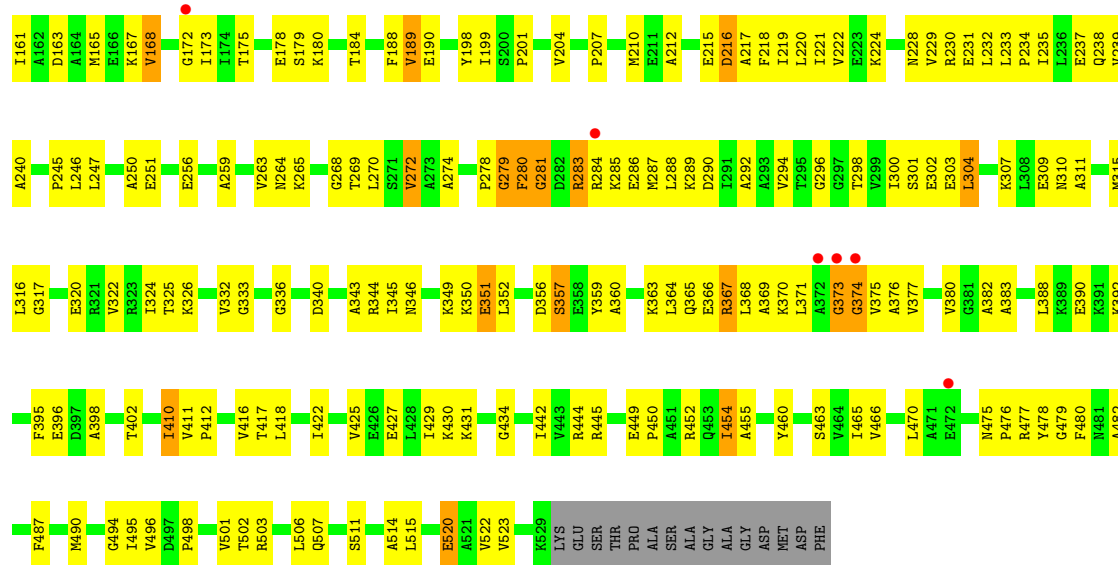
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: cpn60(GroEL)

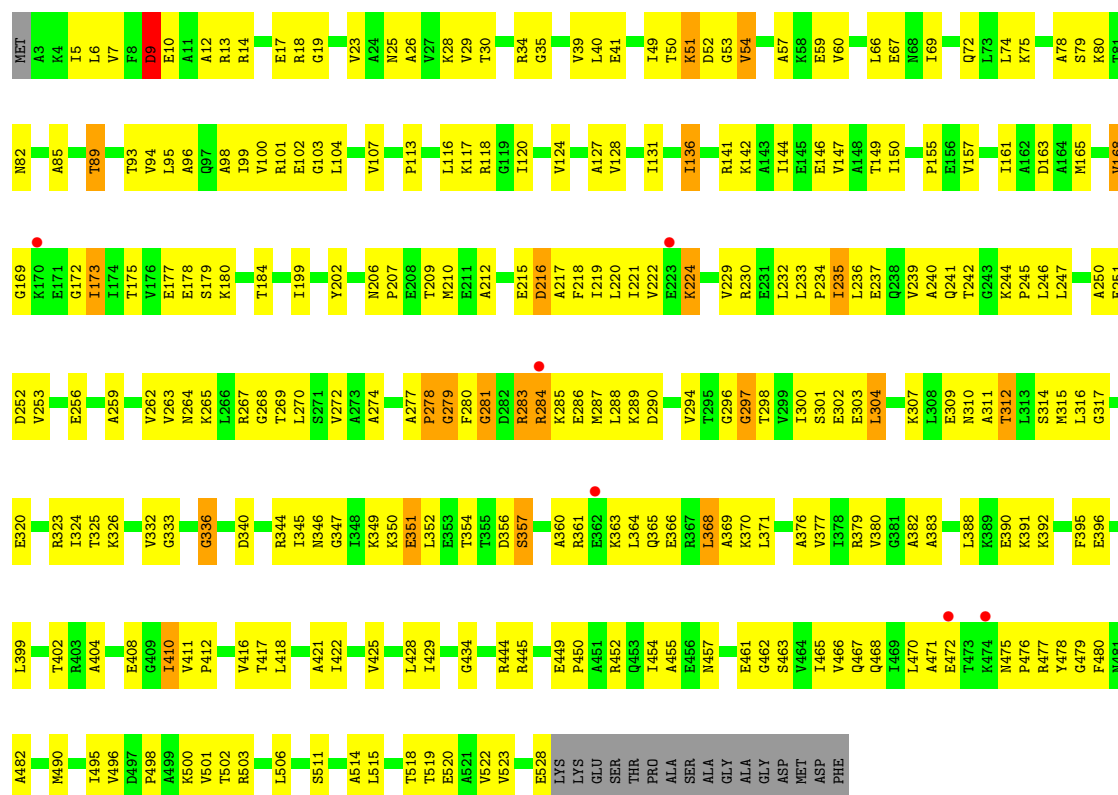


• Molecule 1: cpn60(GroEL)



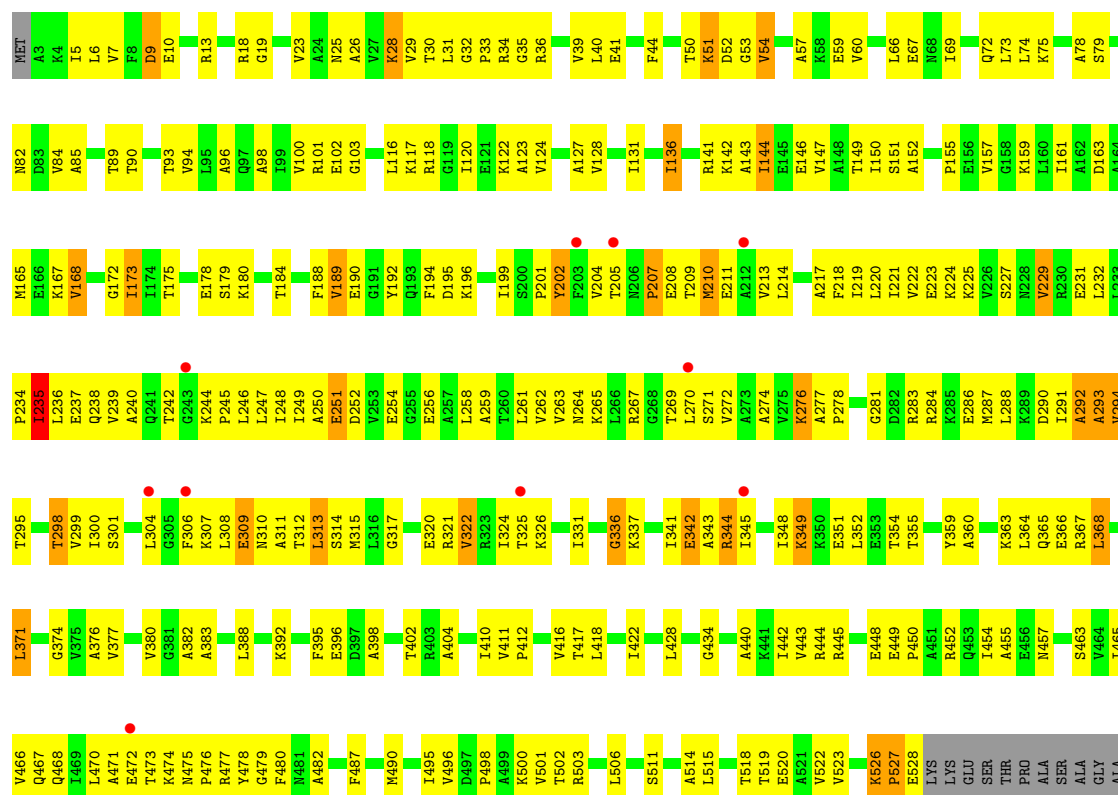


• Molecule 1: cpn60(GroEL)



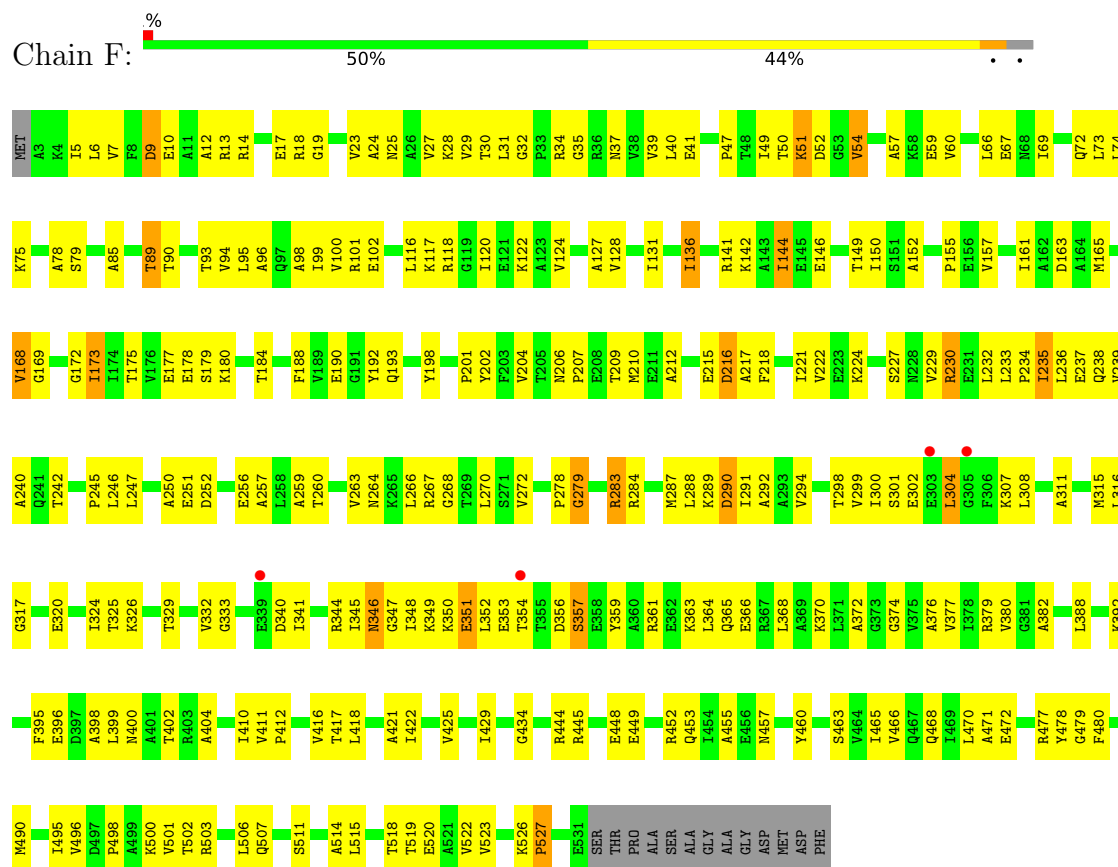
• Molecule 1: cpn60(GroEL)



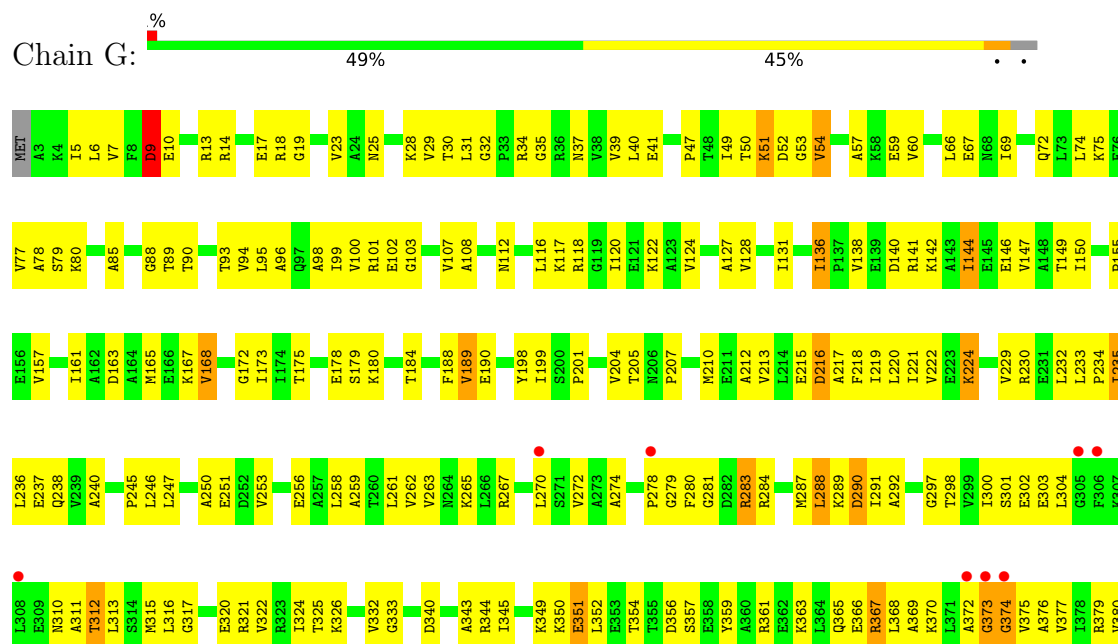


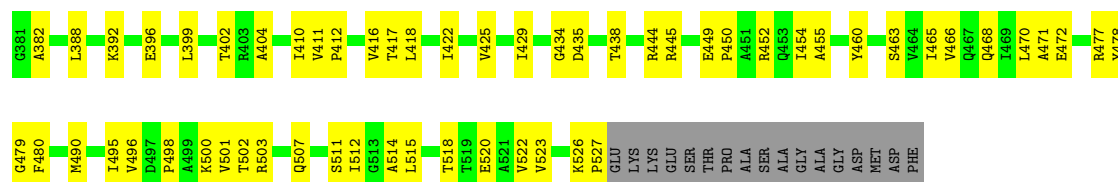
GLY
ASP
MET
ASP
PHE

• Molecule 1: cpn60(GroEL)

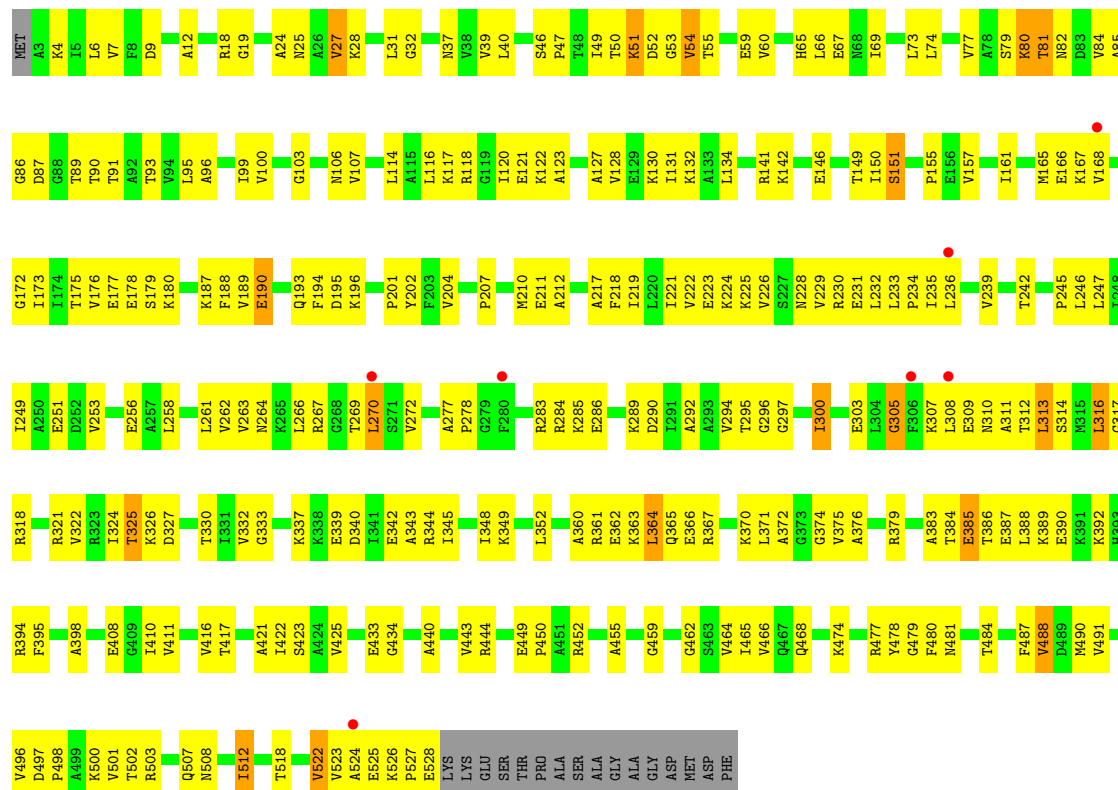


• Molecule 1: cpn60(GroEL)

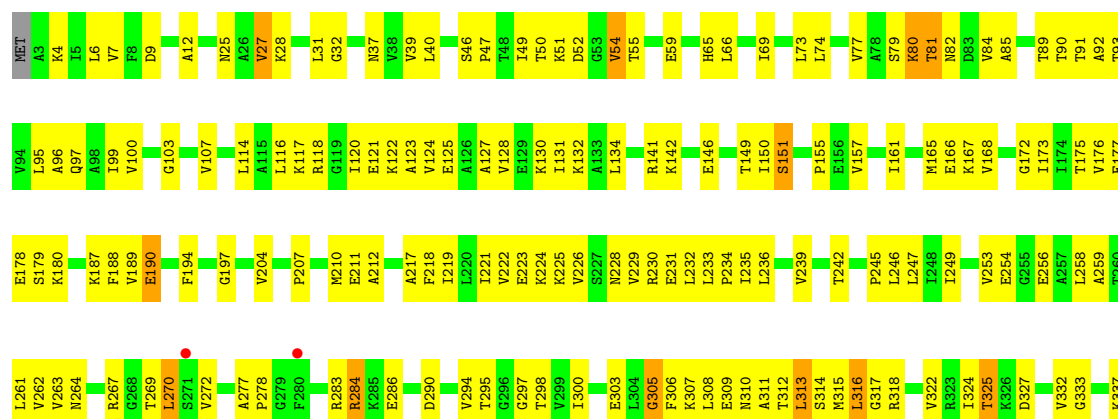


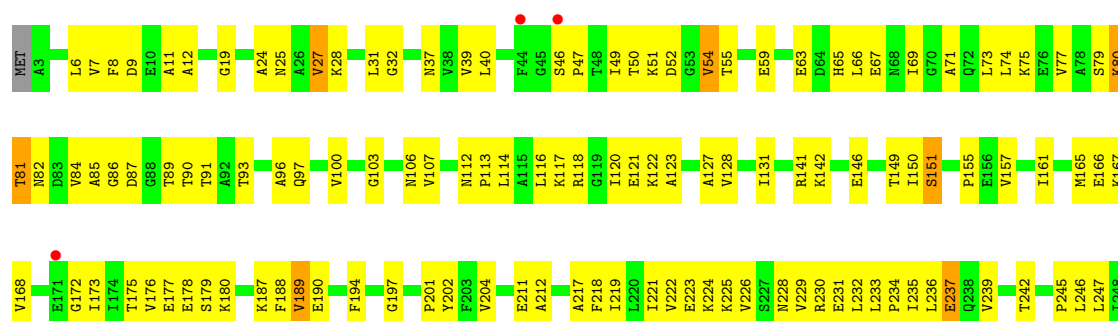


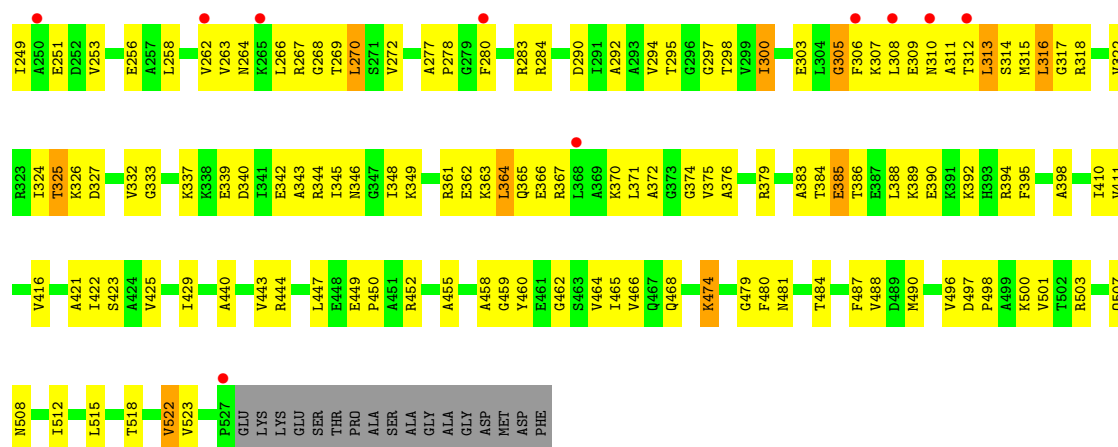
• Molecule 1: cpn60(GroEL)



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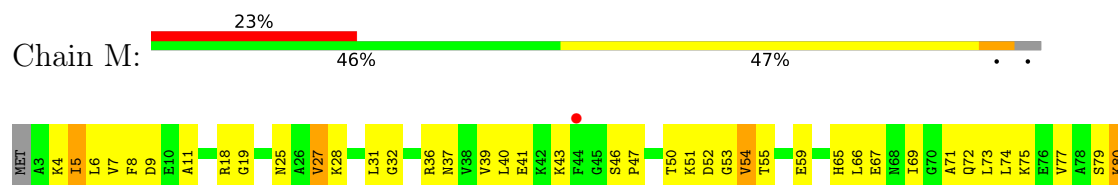


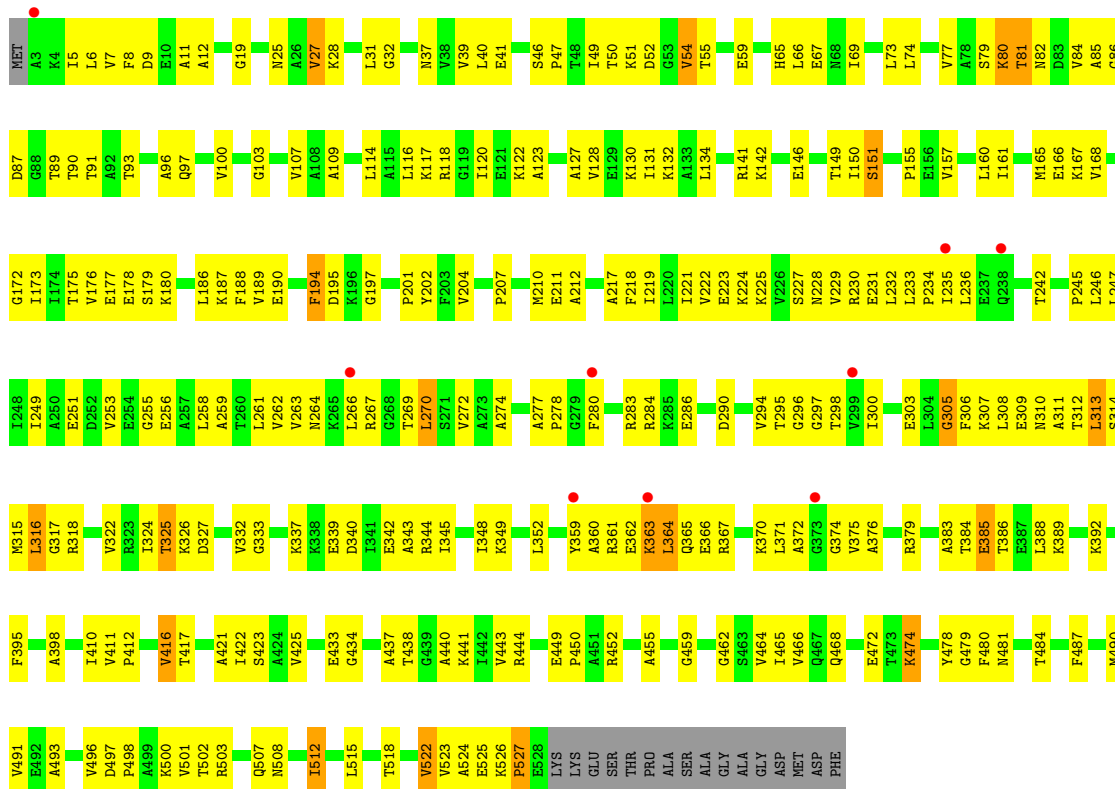


• Molecule 1: cpn60(GroEL)



• Molecule 1: cpn60(GroEL)

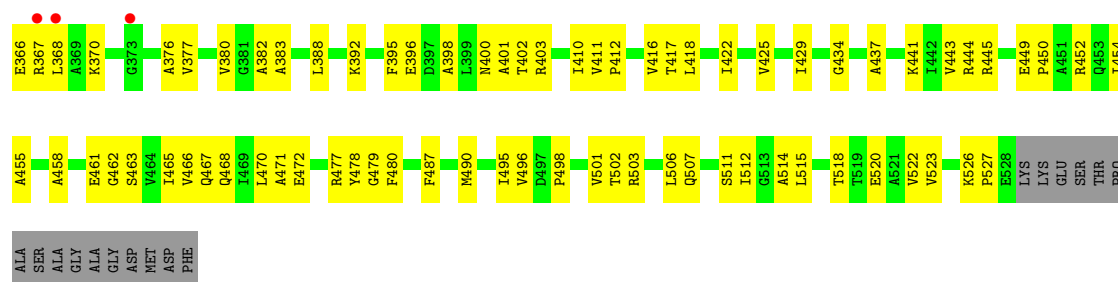




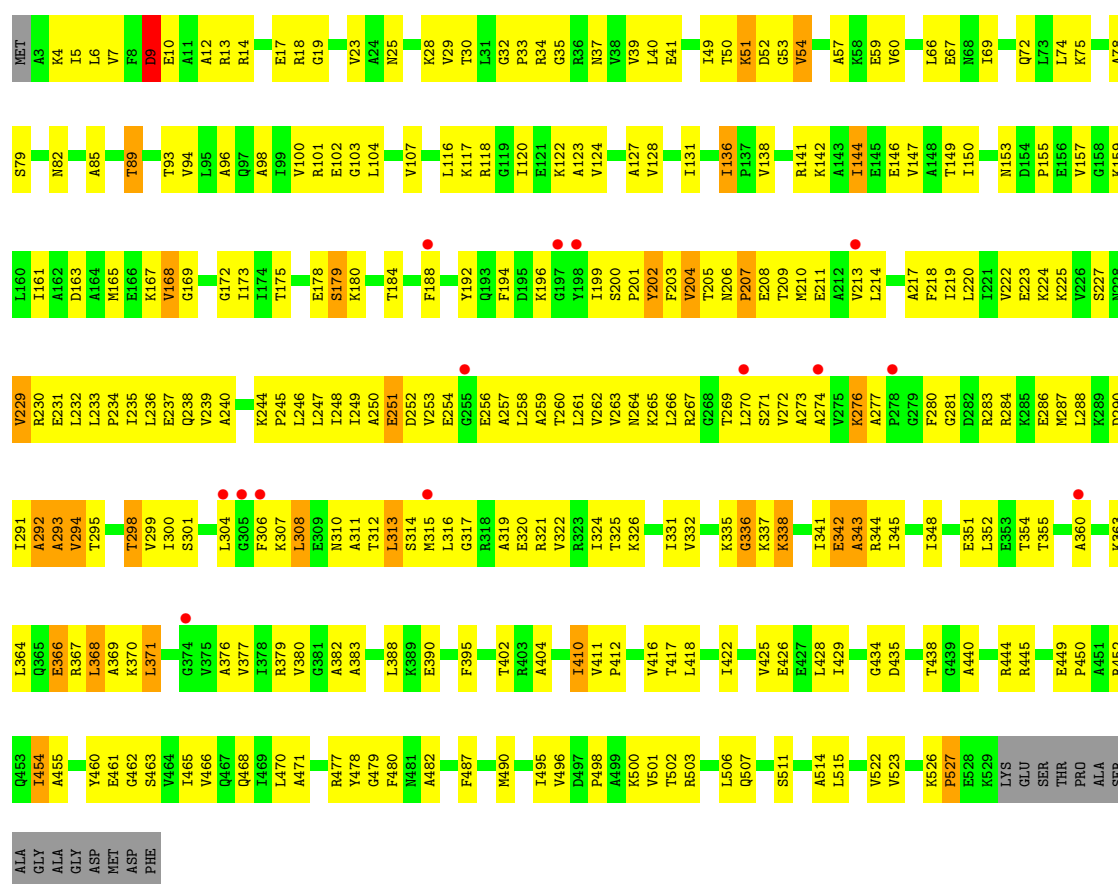
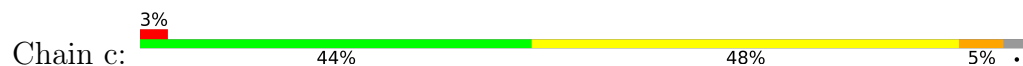
[illegible]

Chain b:

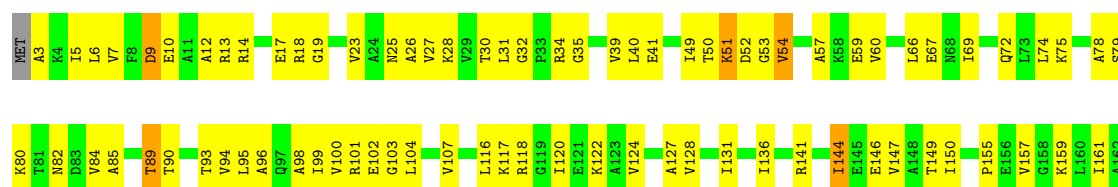
7% 46% 47%

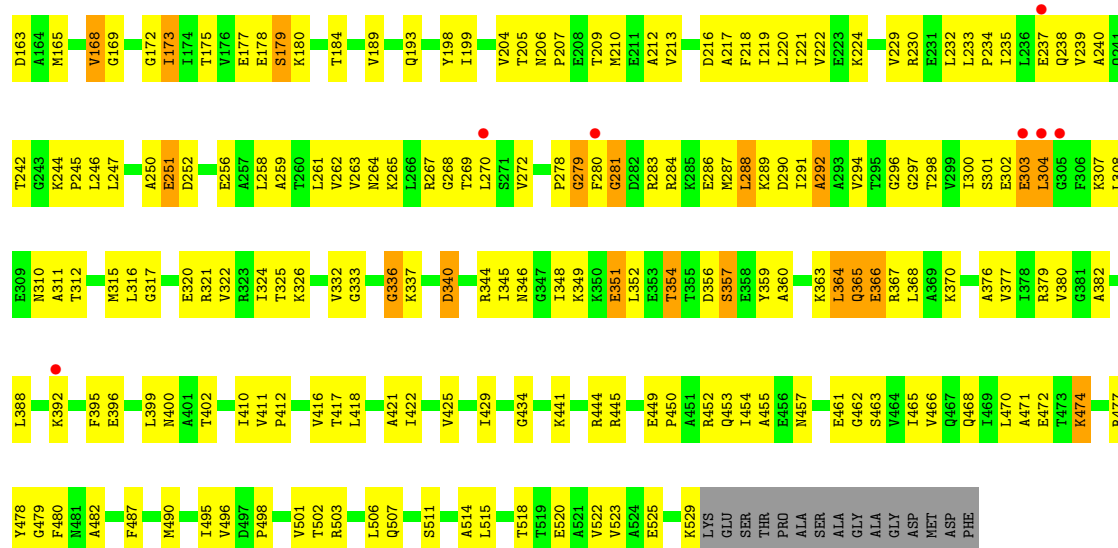


• Molecule 1: cpn60(GroEL)

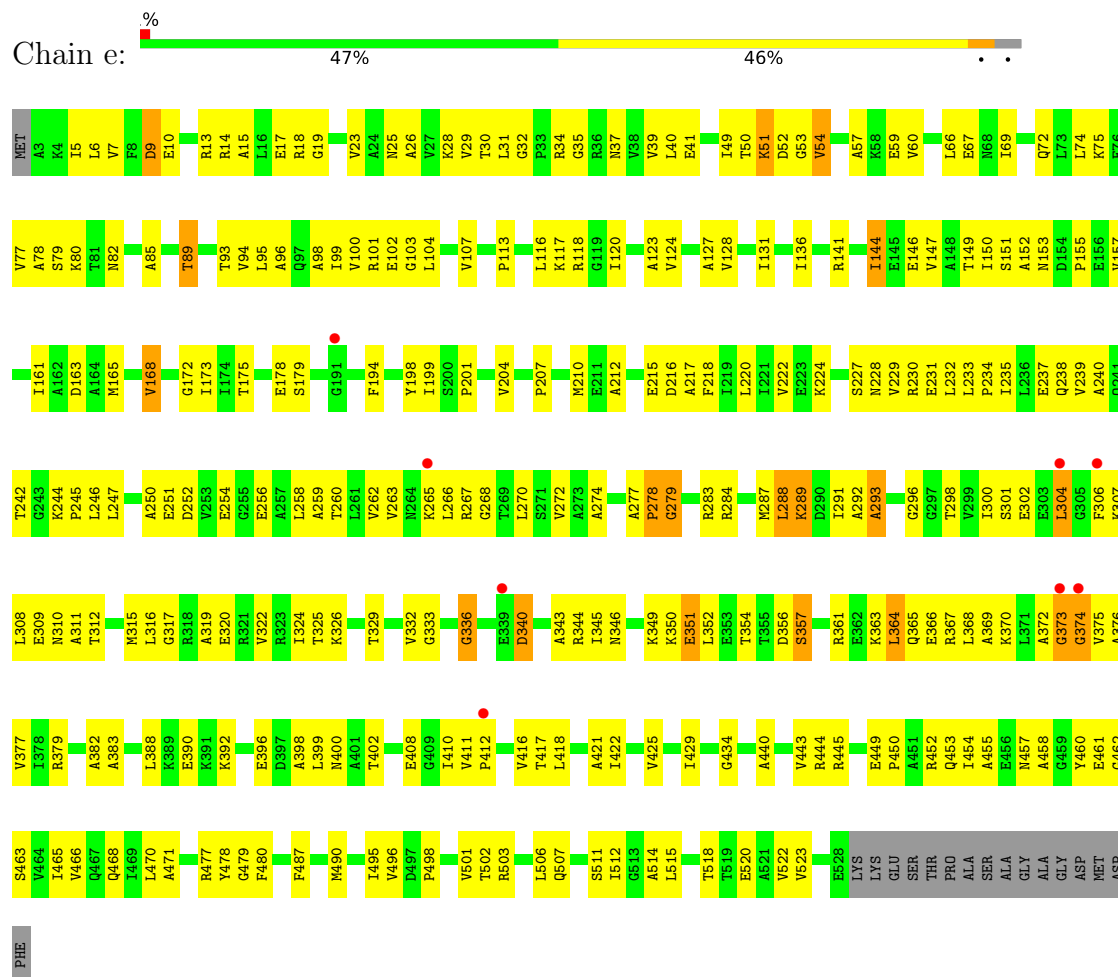


• Molecule 1: cpn60(GroEL)



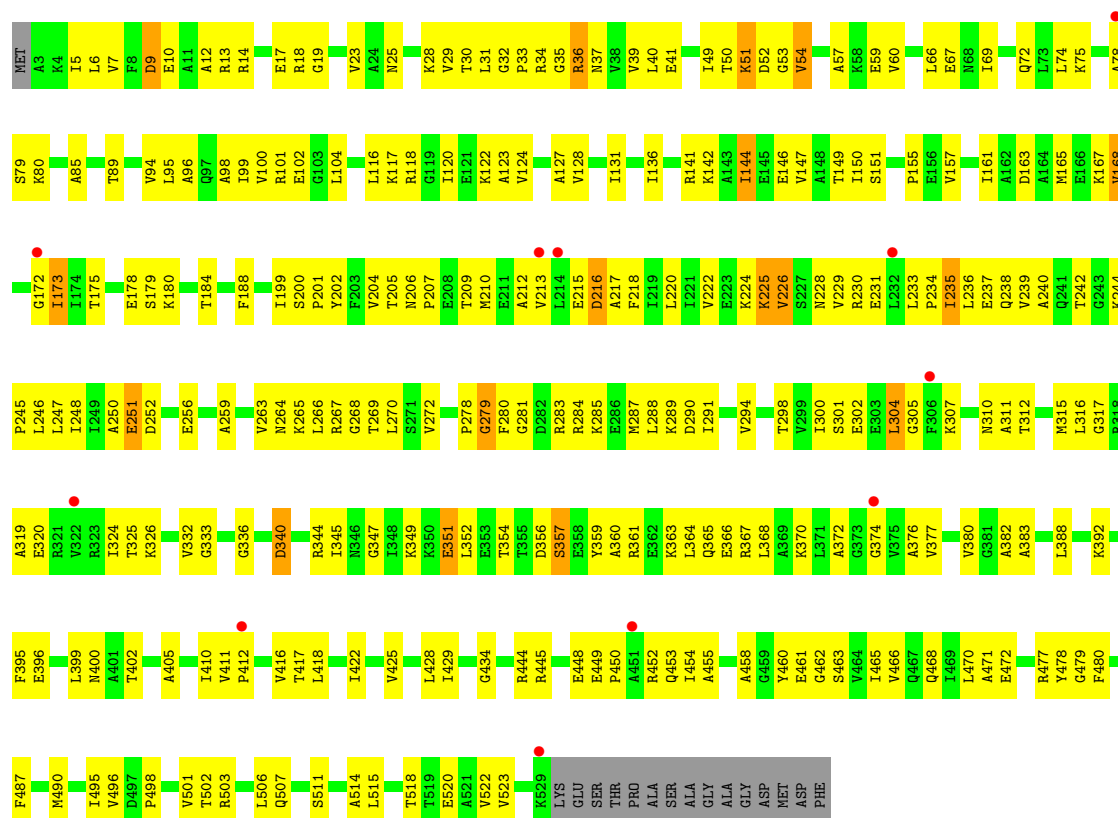


• Molecule 1: cpn60(GroEL)

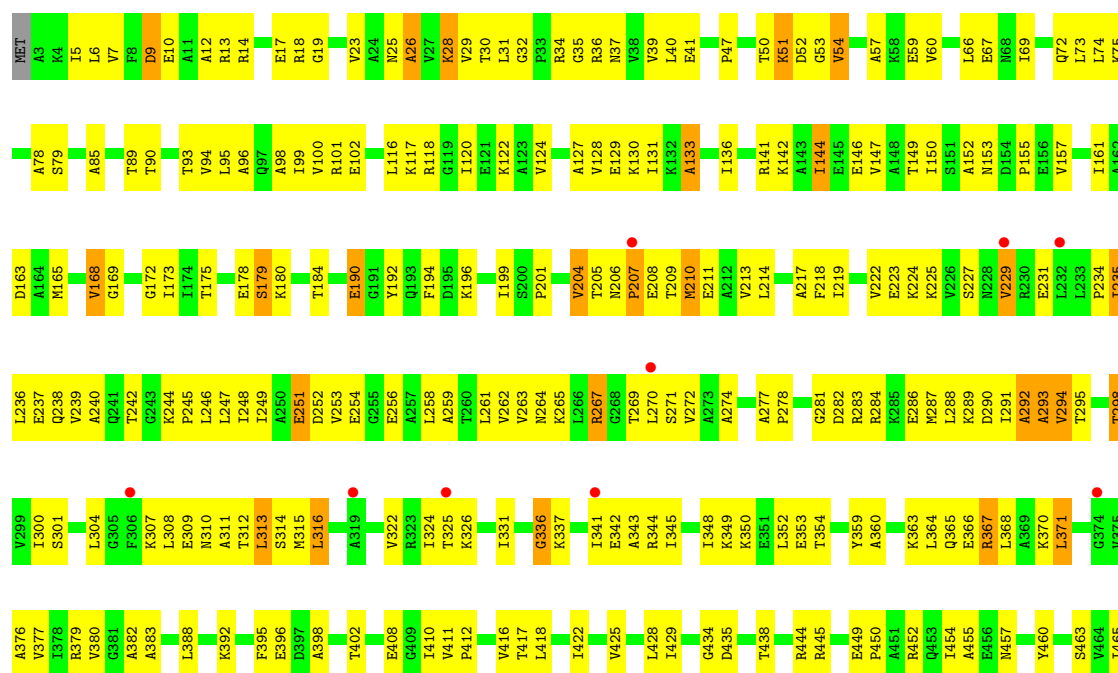


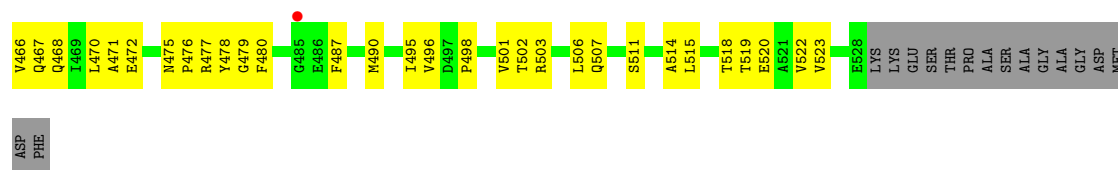
• Molecule 1: cpn60(GroEL)



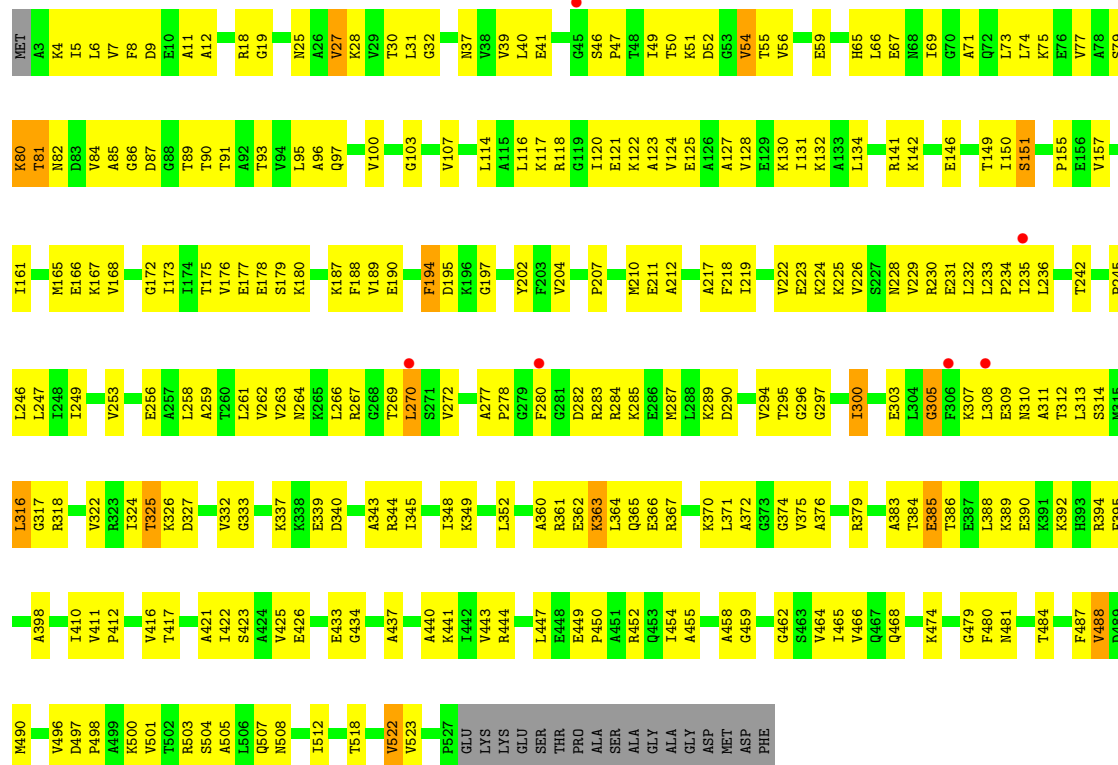


● Molecule 1: cpn60(GroEL)

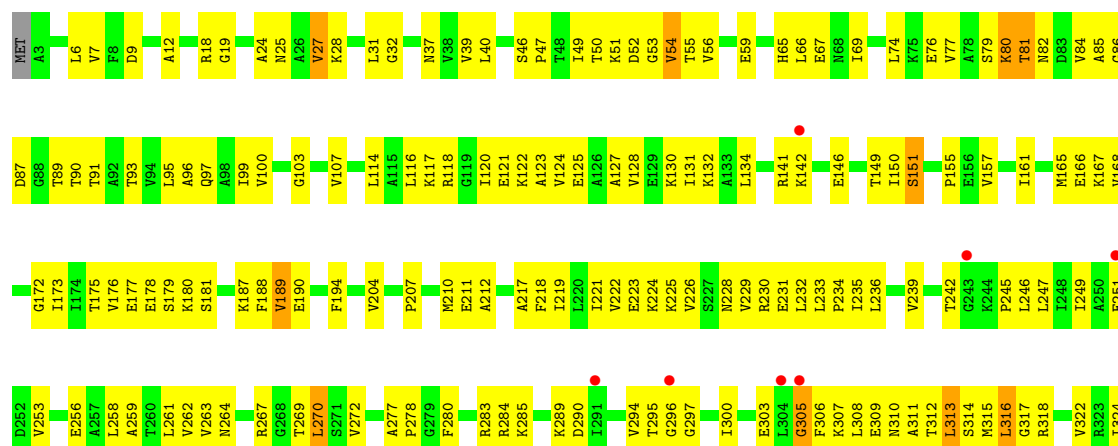


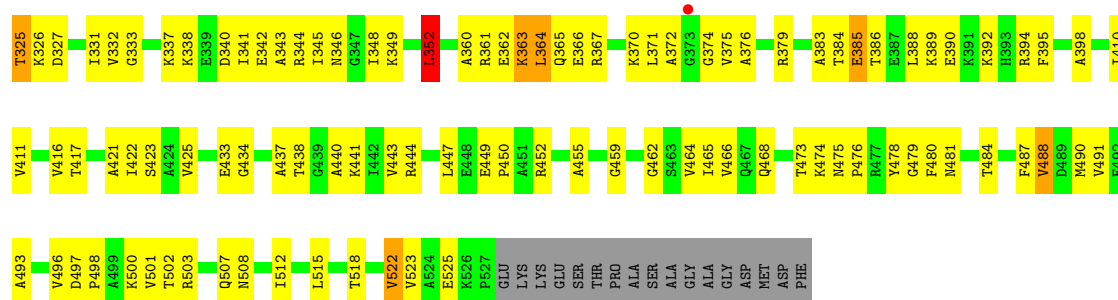


• Molecule 1: cpn60(GroEL)

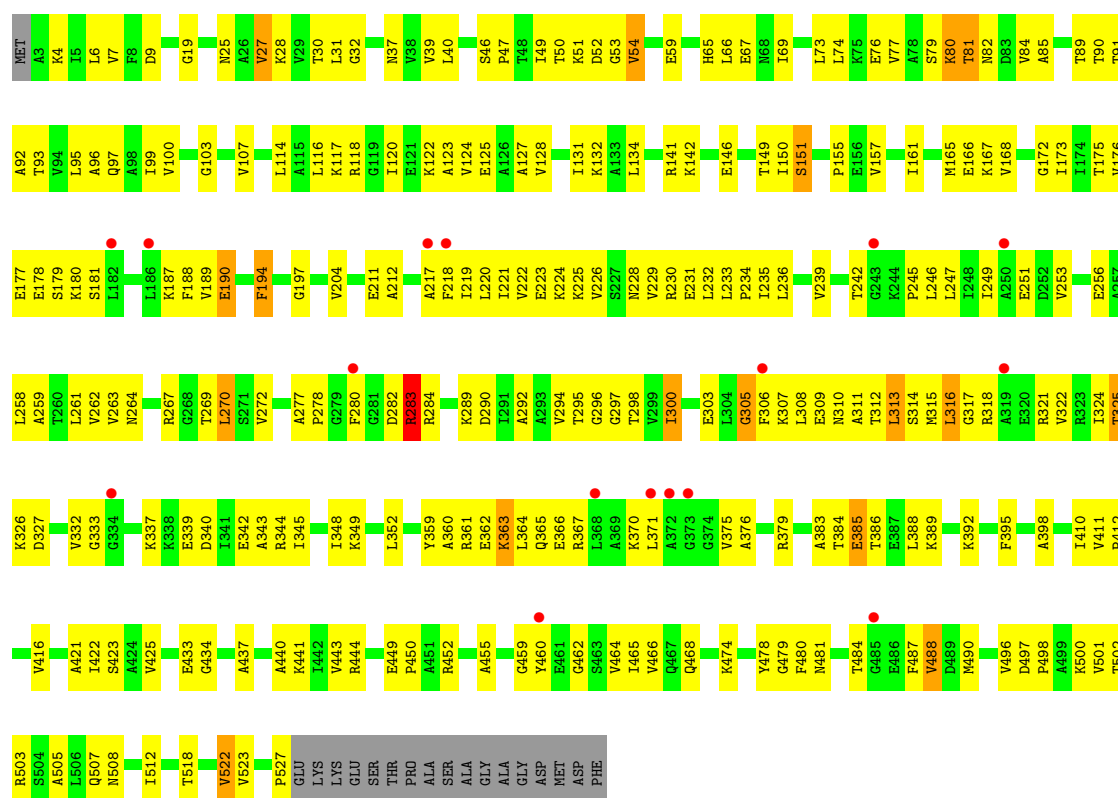


• Molecule 1: cpn60(GroEL)

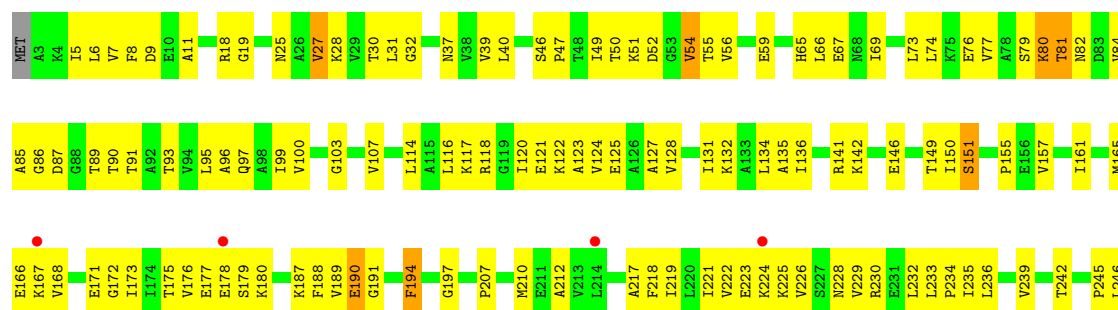


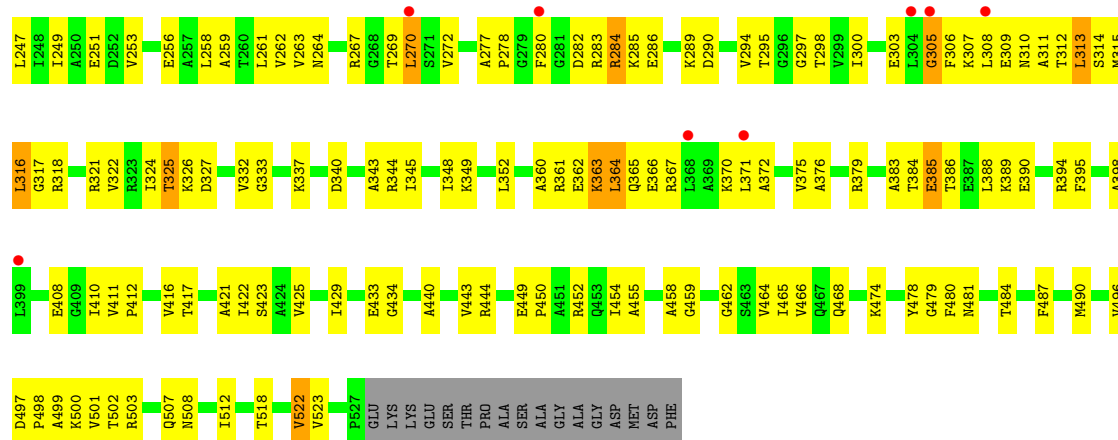


• Molecule 1: cpn60(GroEL)

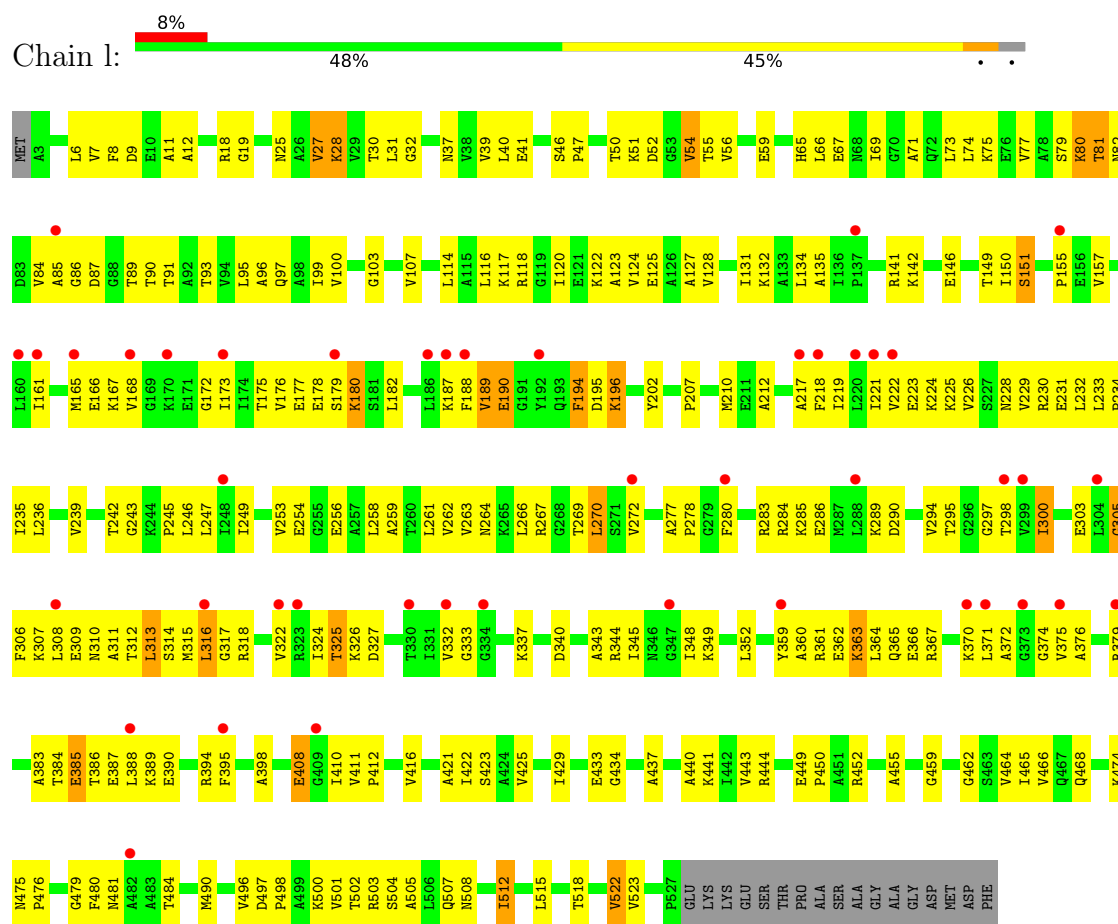


• Molecule 1: cpn60(GroEL)

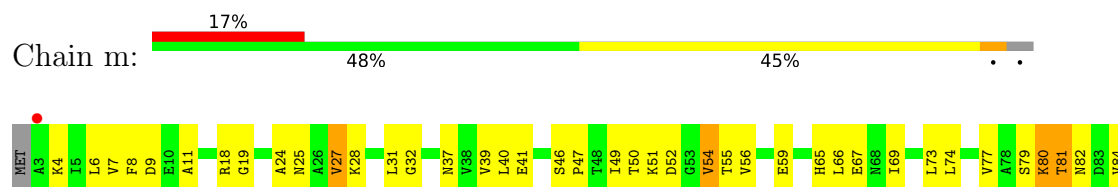


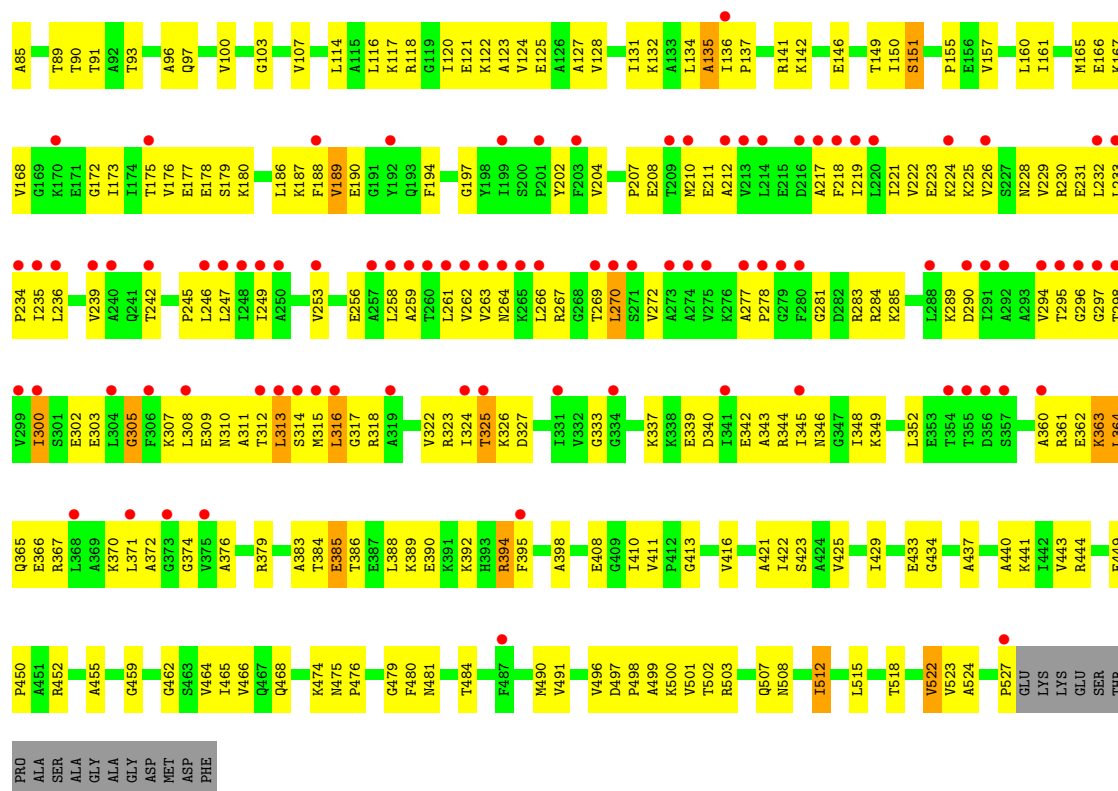


• Molecule 1: cpn60(GroEL)

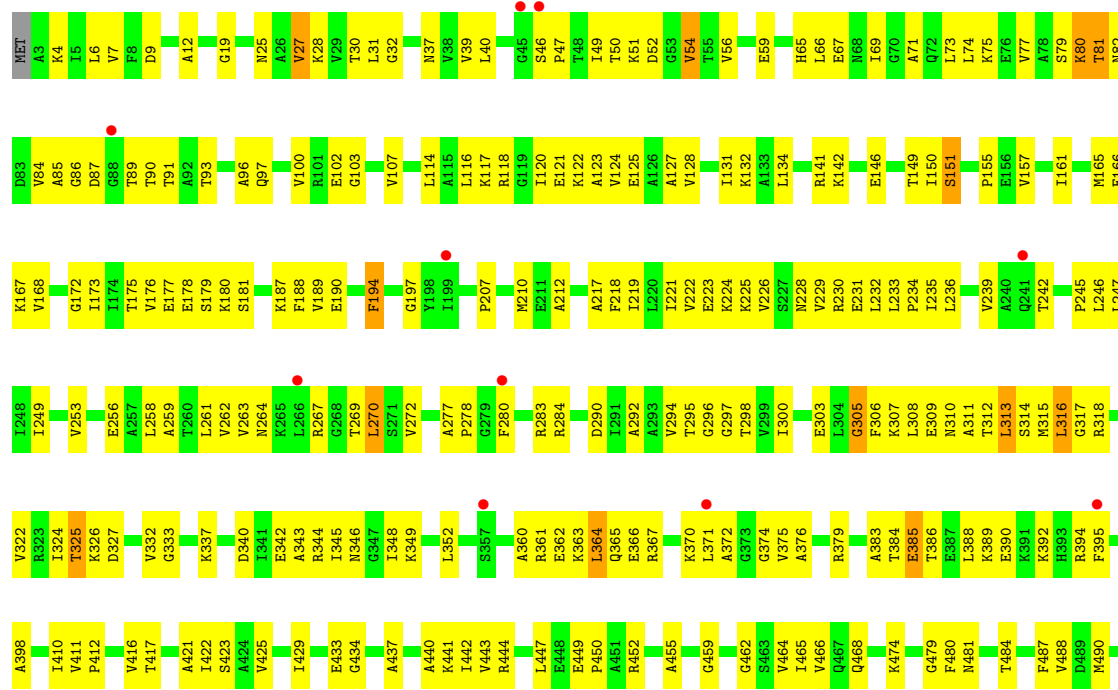


• Molecule 1: cpn60(GroEL)



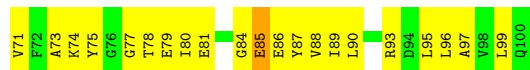
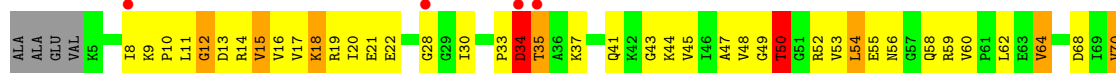


• Molecule 1: cpn60(GroEL)

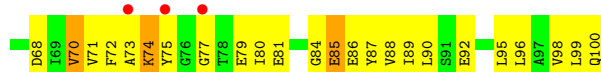
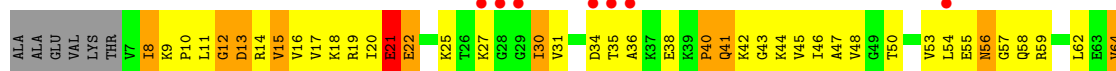




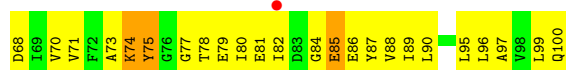
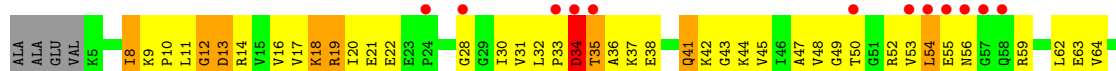
• Molecule 2: cpn10(GroES)



• Molecule 2: cpn10(GroES)



• Molecule 2: cpn10(GroES)

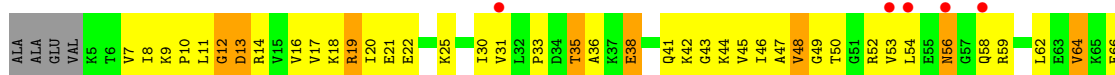


• Molecule 2: cpn10(GroES)

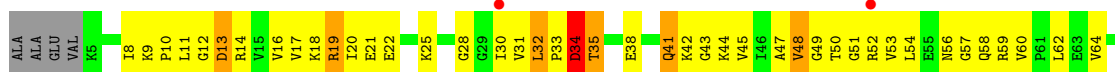


• Molecule 2: cpn10(GroES)





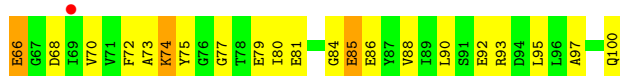
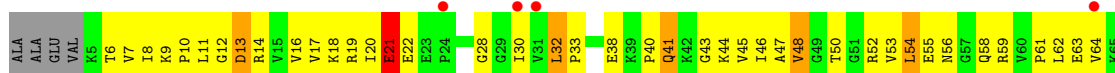
• Molecule 2: cpn10(GroES)



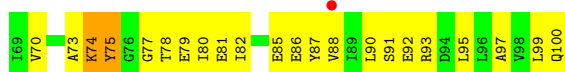
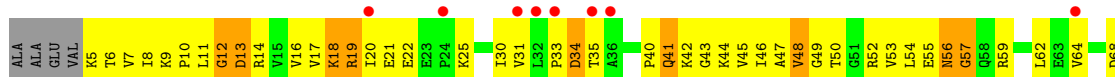
• Molecule 2: cpn10(GroES)



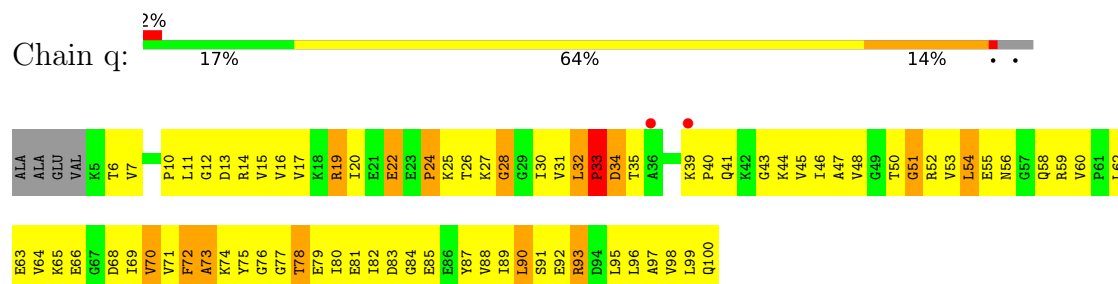
• Molecule 2: cpn10(GroES)



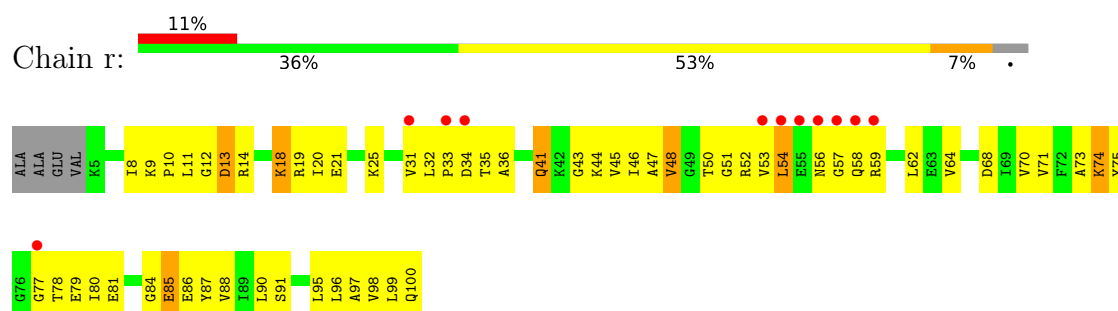
• Molecule 2: cpn10(GroES)



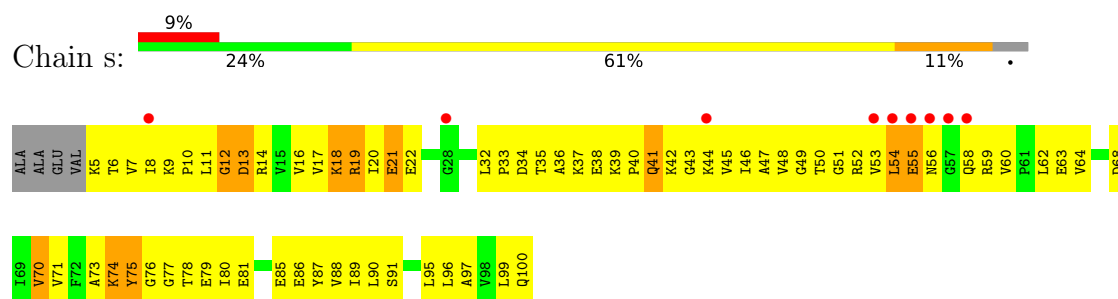
- Molecule 2: cpn10(GroES)



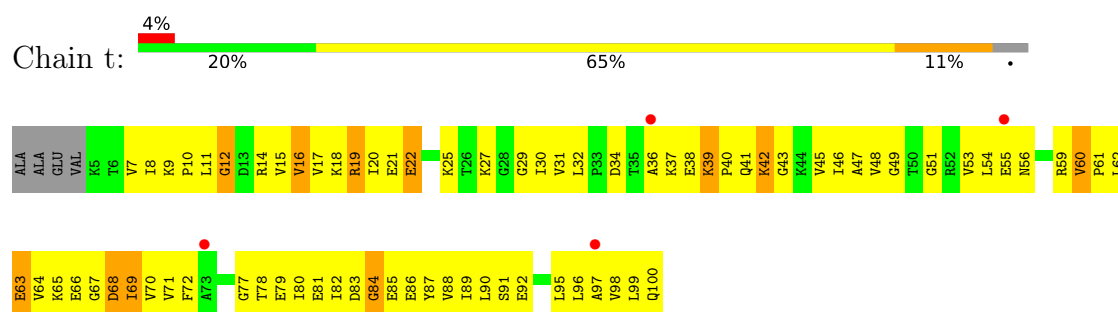
- Molecule 2: cpn10(GroES)



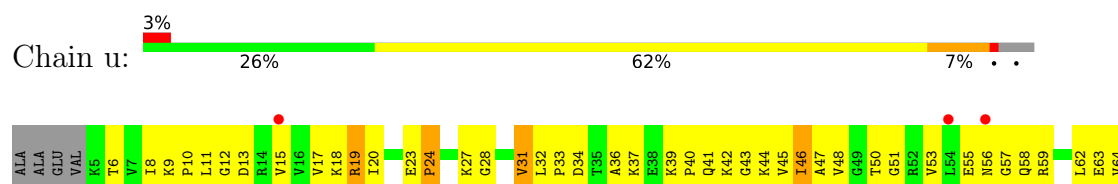
- Molecule 2: cpn10(GroES)



- Molecule 2: cpn10(GroES)



- Molecule 2: cpn10(GroES)



K65	E66	G67	D68	I69	Y70	V71	F72	A73	K74	Y75	T78	E79	I80	E81	I82	E85	E86	Y87	V88	I89	L90	S91	E92	R93	D94	L95	L96	A97	V98	L99	Q100
-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	-----	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	140.38Å 156.42Å 273.15Å 82.88° 85.35° 68.52°	Depositor
Resolution (Å)	39.98 – 2.80 39.98 – 2.80	Depositor EDS
% Data completeness (in resolution range)	81.3 (39.98-2.80) 81.4 (39.98-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.35 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.279 0.239 , 0.278	Depositor DCC
R_{free} test set	12690 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	55.6	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 75.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	121267	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

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

¹Intensities estimated from amplitudes.

²Theoretical 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 ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.58	1/3989 (0.0%)	0.99	10/5383 (0.2%)
1	B	0.54	0/3989	0.98	10/5383 (0.2%)
1	C	0.56	0/3980	1.01	10/5372 (0.2%)
1	D	0.54	0/3980	0.99	13/5372 (0.2%)
1	E	0.55	0/3980	0.99	15/5372 (0.3%)
1	F	0.50	0/4007	0.95	9/5406 (0.2%)
1	G	0.51	0/3971	0.96	8/5360 (0.1%)
1	H	0.44	0/3980	0.94	13/5372 (0.2%)
1	I	0.47	0/3971	0.94	10/5360 (0.2%)
1	J	0.51	0/3971	0.97	11/5360 (0.2%)
1	K	0.49	0/3971	0.96	10/5360 (0.2%)
1	L	0.48	0/3980	0.94	11/5372 (0.2%)
1	M	0.49	0/3971	0.97	13/5360 (0.2%)
1	N	0.47	0/3980	0.97	13/5372 (0.2%)
1	a	0.49	0/3989	0.98	9/5383 (0.2%)
1	b	0.50	0/3980	0.98	9/5372 (0.2%)
1	c	0.47	0/3989	0.99	12/5383 (0.2%)
1	d	0.46	0/3989	0.96	10/5383 (0.2%)
1	e	0.44	0/3980	0.96	9/5372 (0.2%)
1	f	0.41	0/3989	0.94	8/5383 (0.1%)
1	g	0.52	1/3980 (0.0%)	0.95	13/5372 (0.2%)
1	h	0.49	0/3971	0.97	10/5360 (0.2%)
1	i	0.45	1/3971 (0.0%)	0.94	11/5360 (0.2%)
1	j	0.42	0/3971	0.95	11/5360 (0.2%)
1	k	0.41	0/3971	0.94	14/5360 (0.3%)
1	l	0.40	0/3971	0.93	11/5360 (0.2%)
1	m	0.43	1/3971 (0.0%)	0.95	11/5360 (0.2%)
1	n	0.41	0/3971	0.94	10/5360 (0.2%)
2	O	0.48	0/746	1.00	4/1003 (0.4%)
2	P	0.66	1/730 (0.1%)	1.12	6/982 (0.6%)
2	Q	0.48	0/746	0.99	4/1003 (0.4%)
2	R	0.49	0/746	1.07	4/1003 (0.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
2	S	0.47	0/746	1.07	5/1003 (0.5%)
2	T	0.45	0/746	1.00	2/1003 (0.2%)
2	U	0.50	0/746	1.04	2/1003 (0.2%)
2	o	0.53	0/746	1.06	4/1003 (0.4%)
2	p	0.45	0/746	1.06	3/1003 (0.3%)
2	q	0.47	0/746	0.98	0/1003
2	r	0.49	0/746	1.00	1/1003 (0.1%)
2	s	0.60	0/746	1.07	5/1003 (0.5%)
2	t	0.41	0/746	0.94	3/1003 (0.3%)
2	u	0.37	0/746	0.98	2/1003 (0.2%)
All	All	0.48	5/121841 (0.0%)	0.97	349/164393 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	133	ALA	CA-CB	-17.13	1.24	1.53
1	m	394	ARG	CZ-NH2	-9.24	1.21	1.33
1	A	528	GLU	CA-C	6.71	1.61	1.52
1	i	352	LEU	CG-CD2	-5.85	1.33	1.52
2	P	40	PRO	C-O	-5.07	1.17	1.23

The worst 5 of 349 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	27	VAL	N-CA-C	9.38	119.35	110.53
1	m	81	THR	N-CA-C	-8.89	102.35	113.55
2	u	23	GLU	CA-C-N	8.88	130.94	119.84
2	u	23	GLU	C-N-CA	8.88	130.94	119.84
1	b	268	GLY	N-CA-C	-8.85	102.47	114.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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	3956	0	4129	247	0
1	B	3956	0	4129	248	0
1	C	3947	0	4116	255	1
1	D	3947	0	4116	273	0
1	E	3947	0	4116	299	3
1	F	3974	0	4148	254	0
1	G	3938	0	4110	233	0
1	H	3947	0	4116	268	0
1	I	3938	0	4110	258	0
1	J	3938	0	4110	279	0
1	K	3938	0	4110	268	1
1	L	3947	0	4116	327	1
1	M	3938	0	4110	387	0
1	N	3947	0	4116	309	4
1	a	3956	0	4129	293	0
1	b	3947	0	4116	274	0
1	c	3956	0	4129	324	0
1	d	3956	0	4129	264	4
1	e	3947	0	4116	262	0
1	f	3956	0	4129	248	0
1	g	3947	0	4116	289	4
1	h	3938	0	4110	276	0
1	i	3938	0	4110	281	0
1	j	3938	0	4110	273	0
1	k	3938	0	4110	279	0
1	l	3938	0	4110	303	0
1	m	3938	0	4110	304	0
1	n	3938	0	4110	266	0
2	O	739	0	786	108	0
2	P	723	0	766	107	0
2	Q	739	0	786	96	0
2	R	739	0	786	91	0
2	S	739	0	786	87	0
2	T	739	0	786	82	0
2	U	739	0	786	88	0
2	o	739	0	786	90	0
2	p	739	0	786	85	0
2	q	739	0	786	139	0
2	r	739	0	786	86	0
2	s	739	0	786	119	0
2	t	739	0	786	131	0
2	u	739	0	786	101	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	a	1	0	0	0	0
3	b	1	0	0	0	0
3	c	1	0	0	0	0
3	d	1	0	0	0	0
3	e	1	0	0	0	0
3	f	1	0	0	0	0
3	g	1	0	0	0	0
4	A	27	0	12	0	0
4	B	27	0	12	0	0
4	C	27	0	12	0	0
4	D	27	0	12	1	0
4	E	27	0	12	2	0
4	F	27	0	12	0	0
4	G	27	0	12	1	0
4	a	27	0	12	1	0
4	b	27	0	12	1	0
4	c	27	0	12	1	0
4	d	27	0	12	0	0
4	e	27	0	12	3	0
4	f	27	0	12	2	0
4	g	27	0	12	0	0
5	H	4	0	6	2	0
5	I	4	0	6	0	0
5	J	4	0	6	0	0
5	K	4	0	6	2	0
5	L	4	0	6	0	0
5	M	4	0	6	0	0
5	N	4	0	6	0	0
5	h	4	0	6	0	0
5	i	4	0	6	0	0
5	j	4	0	6	0	0
5	k	4	0	6	0	0
5	l	4	0	6	0	0
5	m	4	0	6	0	0
5	n	4	0	6	0	0
All	All	121267	0	126522	8582	9

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 35.

The worst 5 of 8582 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:D:150:ILE:HD11	1:D:495:ILE:HA	1.22	1.21
1:d:3:ALA:HB1	1:d:529:LYS:NZ	1.56	1.21
1:k:283:ARG:NH2	1:k:367:ARG:HD3	1.56	1.20
1:k:283:ARG:HH21	1:k:367:ARG:CD	1.55	1.19
1:i:283:ARG:NH2	1:i:367:ARG:HD3	1.56	1.18

The worst 5 of 9 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:474:LYS:CE	1:N:472:GLU:OE1[1_455]	1.85	0.35
1:K:474:LYS:NZ	1:N:493:ALA:O[1_455]	1.93	0.27
1:d:474:LYS:CE	1:g:133:ALA:CB[1_455]	1.93	0.27
1:d:474:LYS:NZ	1:g:133:ALA:CB[1_455]	1.95	0.25
1:C:141:ARG:NH2	1:L:353:GLU:OE1[1_565]	2.11	0.09

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	525/543 (97%)	456 (87%)	56 (11%)	13 (2%)	4	16
1	B	525/543 (97%)	458 (87%)	55 (10%)	12 (2%)	5	18
1	C	524/543 (96%)	451 (86%)	58 (11%)	15 (3%)	3	13
1	D	524/543 (96%)	441 (84%)	67 (13%)	16 (3%)	3	12
1	E	524/543 (96%)	440 (84%)	65 (12%)	19 (4%)	2	10
1	F	527/543 (97%)	453 (86%)	60 (11%)	14 (3%)	4	15

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	523/543 (96%)	447 (86%)	65 (12%)	11 (2%)	5	20
1	H	524/543 (96%)	457 (87%)	60 (12%)	7 (1%)	9	31
1	I	523/543 (96%)	457 (87%)	61 (12%)	5 (1%)	12	38
1	J	523/543 (96%)	456 (87%)	58 (11%)	9 (2%)	7	25
1	K	523/543 (96%)	458 (88%)	57 (11%)	8 (2%)	8	28
1	L	524/543 (96%)	454 (87%)	63 (12%)	7 (1%)	9	31
1	M	523/543 (96%)	455 (87%)	61 (12%)	7 (1%)	9	31
1	N	524/543 (96%)	457 (87%)	61 (12%)	6 (1%)	11	36
1	a	525/543 (97%)	453 (86%)	57 (11%)	15 (3%)	3	13
1	b	524/543 (96%)	452 (86%)	61 (12%)	11 (2%)	5	20
1	c	525/543 (97%)	446 (85%)	61 (12%)	18 (3%)	3	11
1	d	525/543 (97%)	451 (86%)	56 (11%)	18 (3%)	3	11
1	e	524/543 (96%)	455 (87%)	57 (11%)	12 (2%)	5	18
1	f	525/543 (97%)	458 (87%)	55 (10%)	12 (2%)	5	18
1	g	524/543 (96%)	450 (86%)	60 (12%)	14 (3%)	4	15
1	h	523/543 (96%)	459 (88%)	57 (11%)	7 (1%)	9	31
1	i	523/543 (96%)	456 (87%)	58 (11%)	9 (2%)	7	25
1	j	523/543 (96%)	454 (87%)	60 (12%)	9 (2%)	7	25
1	k	523/543 (96%)	456 (87%)	61 (12%)	6 (1%)	11	36
1	l	523/543 (96%)	457 (87%)	59 (11%)	7 (1%)	9	31
1	m	523/543 (96%)	465 (89%)	51 (10%)	7 (1%)	9	31
1	n	523/543 (96%)	459 (88%)	58 (11%)	6 (1%)	11	36
2	O	94/100 (94%)	74 (79%)	13 (14%)	7 (7%)	1	2
2	P	92/100 (92%)	72 (78%)	13 (14%)	7 (8%)	1	2
2	Q	94/100 (94%)	75 (80%)	12 (13%)	7 (7%)	1	2
2	R	94/100 (94%)	75 (80%)	11 (12%)	8 (8%)	0	1
2	S	94/100 (94%)	72 (77%)	17 (18%)	5 (5%)	1	5
2	T	94/100 (94%)	72 (77%)	15 (16%)	7 (7%)	1	2
2	U	94/100 (94%)	77 (82%)	10 (11%)	7 (7%)	1	2
2	o	94/100 (94%)	75 (80%)	13 (14%)	6 (6%)	1	3
2	p	94/100 (94%)	72 (77%)	15 (16%)	7 (7%)	1	2

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	q	94/100 (94%)	58 (62%)	21 (22%)	15 (16%)	0	0
2	r	94/100 (94%)	71 (76%)	17 (18%)	6 (6%)	1	3
2	s	94/100 (94%)	76 (81%)	13 (14%)	5 (5%)	1	5
2	t	94/100 (94%)	69 (73%)	17 (18%)	8 (8%)	0	1
2	u	94/100 (94%)	66 (70%)	18 (19%)	10 (11%)	0	1
All	All	15983/16604 (96%)	13715 (86%)	1863 (12%)	405 (2%)	4	16

5 of 405 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	ASP
1	A	278	PRO
1	B	9	ASP
1	B	278	PRO
1	C	9	ASP

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	412/423 (97%)	402 (98%)	10 (2%)	43	77
1	B	412/423 (97%)	398 (97%)	14 (3%)	32	68
1	C	411/423 (97%)	398 (97%)	13 (3%)	34	70
1	D	411/423 (97%)	399 (97%)	12 (3%)	37	73
1	E	411/423 (97%)	394 (96%)	17 (4%)	27	62
1	F	414/423 (98%)	405 (98%)	9 (2%)	45	78
1	G	410/423 (97%)	398 (97%)	12 (3%)	37	73
1	H	411/423 (97%)	401 (98%)	10 (2%)	43	77
1	I	410/423 (97%)	401 (98%)	9 (2%)	45	78
1	J	410/423 (97%)	400 (98%)	10 (2%)	43	77
1	K	410/423 (97%)	401 (98%)	9 (2%)	45	78

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	411/423 (97%)	402 (98%)	9 (2%)	45	78
1	M	410/423 (97%)	398 (97%)	12 (3%)	37	73
1	N	411/423 (97%)	399 (97%)	12 (3%)	37	73
1	a	412/423 (97%)	401 (97%)	11 (3%)	39	74
1	b	411/423 (97%)	402 (98%)	9 (2%)	45	78
1	c	412/423 (97%)	397 (96%)	15 (4%)	31	66
1	d	412/423 (97%)	400 (97%)	12 (3%)	37	73
1	e	411/423 (97%)	399 (97%)	12 (3%)	37	73
1	f	412/423 (97%)	404 (98%)	8 (2%)	50	81
1	g	411/423 (97%)	399 (97%)	12 (3%)	37	73
1	h	410/423 (97%)	400 (98%)	10 (2%)	43	77
1	i	410/423 (97%)	400 (98%)	10 (2%)	43	77
1	j	410/423 (97%)	398 (97%)	12 (3%)	37	73
1	k	410/423 (97%)	399 (97%)	11 (3%)	39	74
1	l	410/423 (97%)	397 (97%)	13 (3%)	34	70
1	m	410/423 (97%)	399 (97%)	11 (3%)	39	74
1	n	410/423 (97%)	400 (98%)	10 (2%)	43	77
2	O	81/83 (98%)	77 (95%)	4 (5%)	22	55
2	P	79/83 (95%)	75 (95%)	4 (5%)	21	54
2	Q	81/83 (98%)	76 (94%)	5 (6%)	16	45
2	R	81/83 (98%)	79 (98%)	2 (2%)	42	76
2	S	81/83 (98%)	78 (96%)	3 (4%)	30	65
2	T	81/83 (98%)	77 (95%)	4 (5%)	22	55
2	U	81/83 (98%)	77 (95%)	4 (5%)	22	55
2	o	81/83 (98%)	78 (96%)	3 (4%)	30	65
2	p	81/83 (98%)	78 (96%)	3 (4%)	30	65
2	q	81/83 (98%)	77 (95%)	4 (5%)	22	55
2	r	81/83 (98%)	78 (96%)	3 (4%)	30	65
2	s	81/83 (98%)	76 (94%)	5 (6%)	16	45
2	t	81/83 (98%)	78 (96%)	3 (4%)	30	65
2	u	81/83 (98%)	79 (98%)	2 (2%)	42	76

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	12637/13006 (97%)	12274 (97%)	363 (3%)	37 73

5 of 363 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	e	5	ILE
1	j	190	GLU
1	e	266	LEU
1	g	298	THR
1	k	270	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 304 such sidechains are listed below:

Mol	Chain	Res	Type
1	j	228	ASN
1	n	153	ASN
1	j	481	ASN
1	l	193	GLN
2	t	41	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 42 ligands modelled in this entry, 14 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
5	DMS	n	701	-	3,3,3	0.25	0	3,3,3	0.64	0
4	ADP	A	602	3	28,29,29	1.27	3 (10%)	43,45,45	1.81	7 (16%)
4	ADP	F	602	3	28,29,29	1.52	4 (14%)	43,45,45	2.09	11 (25%)
5	DMS	k	601	-	3,3,3	0.31	0	3,3,3	0.68	0
4	ADP	B	602	3	28,29,29	1.44	4 (14%)	43,45,45	2.10	11 (25%)
4	ADP	C	602	3	28,29,29	1.40	3 (10%)	43,45,45	1.96	11 (25%)
4	ADP	e	602	3	28,29,29	1.61	7 (25%)	43,45,45	2.17	11 (25%)
4	ADP	b	602	3	28,29,29	1.45	5 (17%)	43,45,45	1.98	8 (18%)
4	ADP	c	602	3	28,29,29	1.64	6 (21%)	43,45,45	2.32	11 (25%)
5	DMS	J	601	-	3,3,3	0.38	0	3,3,3	0.77	0
4	ADP	d	602	3	28,29,29	1.60	5 (17%)	43,45,45	2.08	12 (27%)
4	ADP	D	602	3	28,29,29	1.52	7 (25%)	43,45,45	1.94	8 (18%)
5	DMS	K	601	-	3,3,3	0.29	0	3,3,3	0.70	0
5	DMS	L	601	-	3,3,3	0.31	0	3,3,3	0.71	0
4	ADP	E	602	3	28,29,29	1.32	5 (17%)	43,45,45	2.07	10 (23%)
5	DMS	I	601	-	3,3,3	0.26	0	3,3,3	0.69	0
4	ADP	g	602	3	28,29,29	1.55	4 (14%)	43,45,45	2.07	11 (25%)
5	DMS	H	601	-	3,3,3	0.22	0	3,3,3	0.68	0
4	ADP	f	602	3	28,29,29	1.48	5 (17%)	43,45,45	2.07	8 (18%)
4	ADP	G	602	3	28,29,29	1.40	6 (21%)	43,45,45	2.06	9 (20%)
5	DMS	i	601	-	3,3,3	0.33	0	3,3,3	0.73	0
5	DMS	j	601	-	3,3,3	0.29	0	3,3,3	0.68	0
5	DMS	l	601	-	3,3,3	0.33	0	3,3,3	0.69	0
5	DMS	M	601	-	3,3,3	0.28	0	3,3,3	0.66	0
4	ADP	a	602	3	28,29,29	1.45	5 (17%)	43,45,45	2.03	9 (20%)
5	DMS	N	701	-	3,3,3	0.25	0	3,3,3	0.67	0
5	DMS	m	601	-	3,3,3	0.26	0	3,3,3	0.63	0
5	DMS	h	601	-	3,3,3	0.35	0	3,3,3	0.72	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
4	ADP	C	602	3	-	7/16/32/32	0/3/3/3
4	ADP	e	602	3	-	7/16/32/32	0/3/3/3
4	ADP	b	602	3	-	8/16/32/32	0/3/3/3
4	ADP	f	602	3	-	8/16/32/32	0/3/3/3
4	ADP	A	602	3	-	6/16/32/32	0/3/3/3
4	ADP	c	602	3	-	8/16/32/32	0/3/3/3
4	ADP	F	602	3	-	7/16/32/32	0/3/3/3
4	ADP	a	602	3	-	7/16/32/32	0/3/3/3
4	ADP	E	602	3	-	8/16/32/32	0/3/3/3
4	ADP	G	602	3	-	7/16/32/32	0/3/3/3
4	ADP	g	602	3	-	8/16/32/32	0/3/3/3
4	ADP	d	602	3	-	6/16/32/32	0/3/3/3
4	ADP	D	602	3	-	8/16/32/32	0/3/3/3
4	ADP	B	602	3	-	7/16/32/32	0/3/3/3

The worst 5 of 69 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	602	ADP	C5-N7	-4.34	1.31	1.39
4	c	602	ADP	C4-N9	-4.20	1.29	1.37
4	g	602	ADP	C5-N7	-4.08	1.31	1.39
4	d	602	ADP	C5-N7	-3.74	1.32	1.39
4	B	602	ADP	C5-N7	-3.68	1.32	1.39

The worst 5 of 137 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	c	602	ADP	N3-C2-N1	-7.32	117.50	128.58
4	f	602	ADP	N3-C2-N1	-7.17	117.72	128.58
4	b	602	ADP	N3-C2-N1	-7.15	117.77	128.58
4	d	602	ADP	N3-C2-N1	-7.14	117.78	128.58
4	C	602	ADP	N3-C2-N1	-7.08	117.86	128.58

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	602	ADP	C5'-O5'-PA-O1A
4	A	602	ADP	C5'-O5'-PA-O2A

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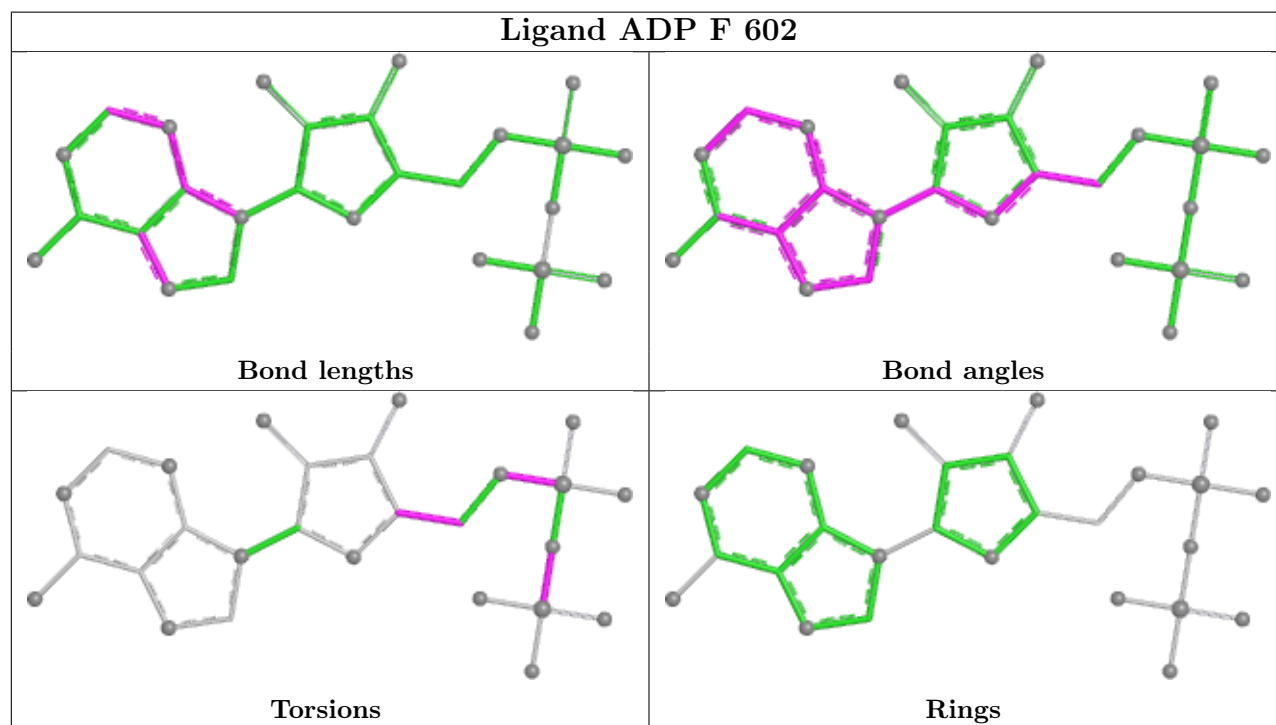
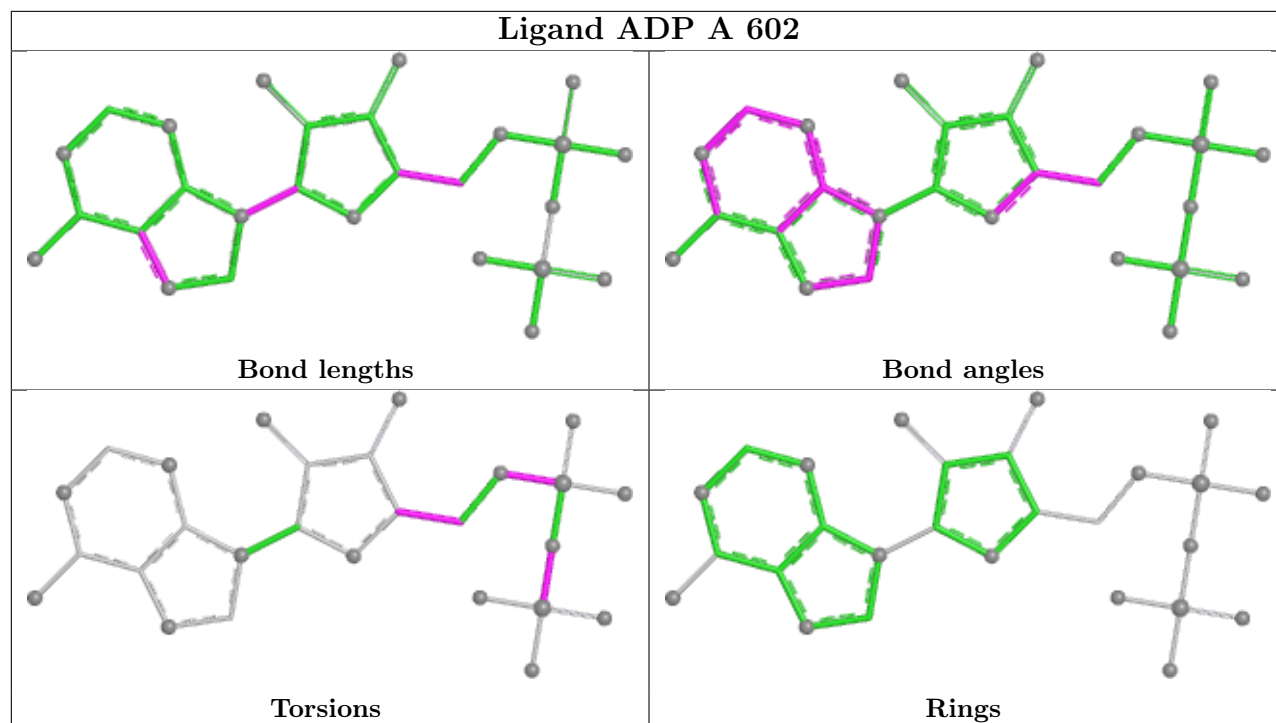
Mol	Chain	Res	Type	Atoms
4	A	602	ADP	C5'-O5'-PA-O3A
4	A	602	ADP	O4'-C4'-C5'-O5'
4	B	602	ADP	C5'-O5'-PA-O1A

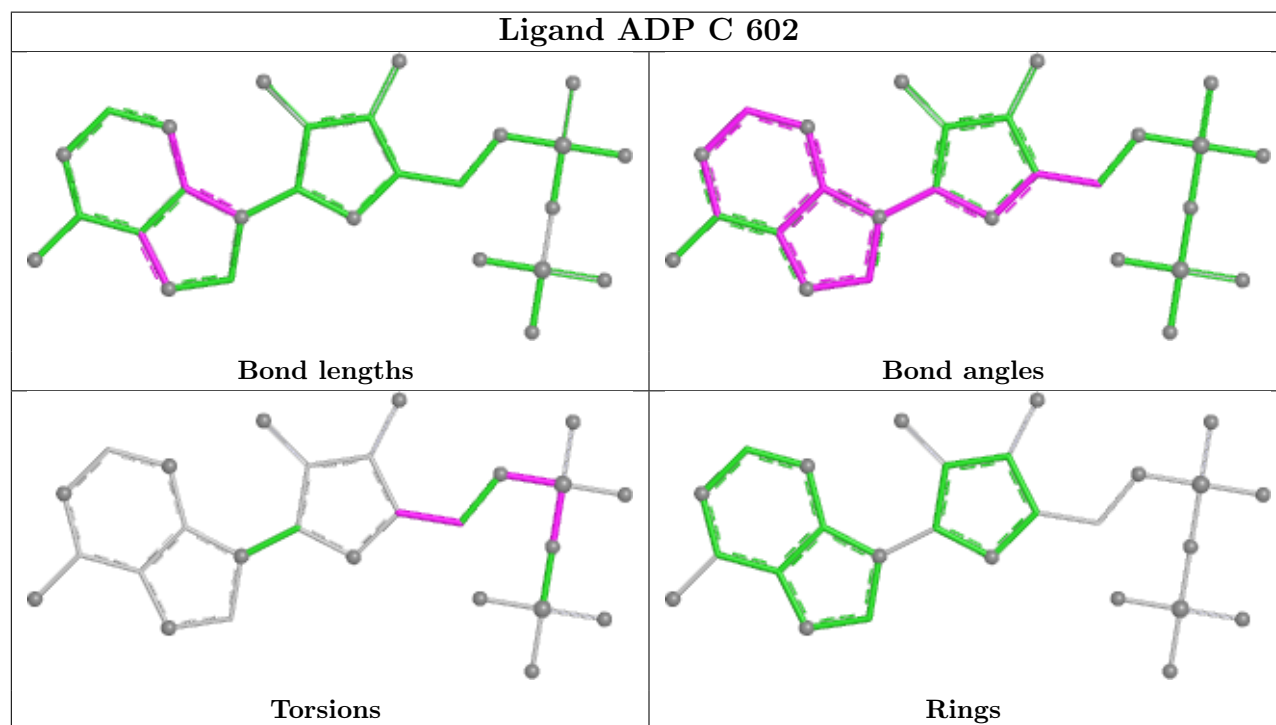
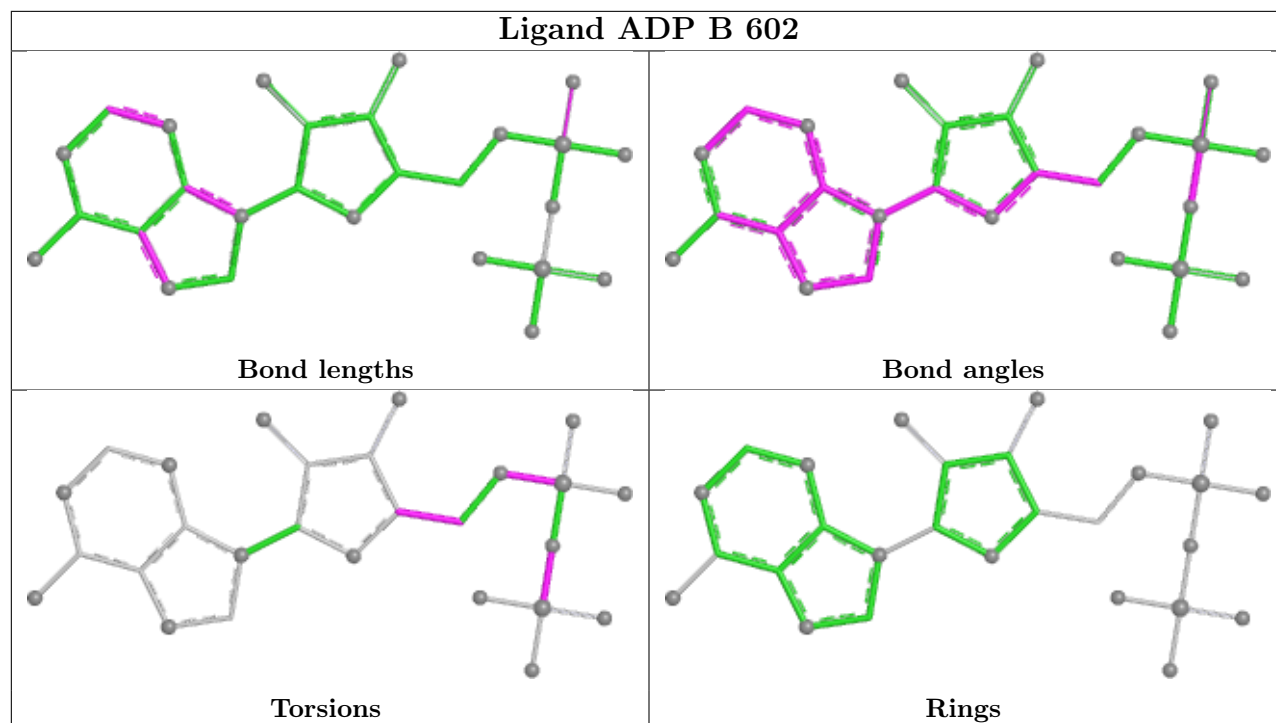
There are no ring outliers.

10 monomers are involved in 16 short contacts:

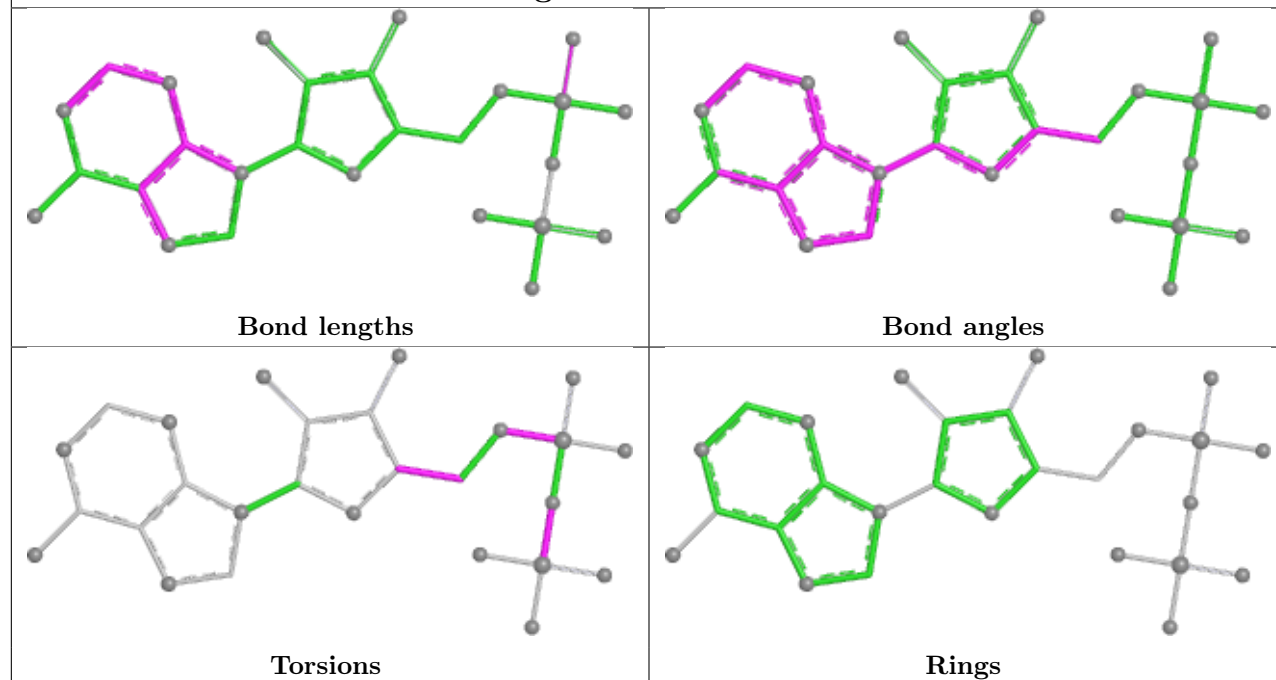
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	e	602	ADP	3	0
4	b	602	ADP	1	0
4	c	602	ADP	1	0
4	D	602	ADP	1	0
5	K	601	DMS	2	0
4	E	602	ADP	2	0
5	H	601	DMS	2	0
4	f	602	ADP	2	0
4	G	602	ADP	1	0
4	a	602	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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.

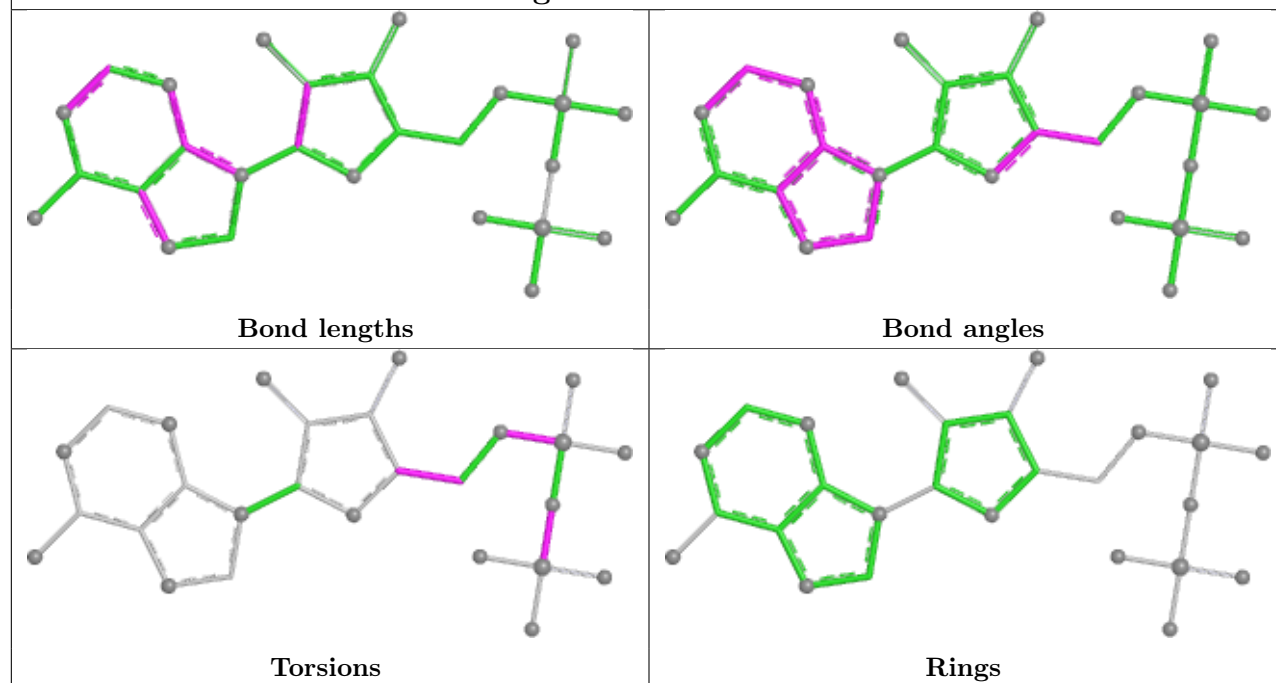




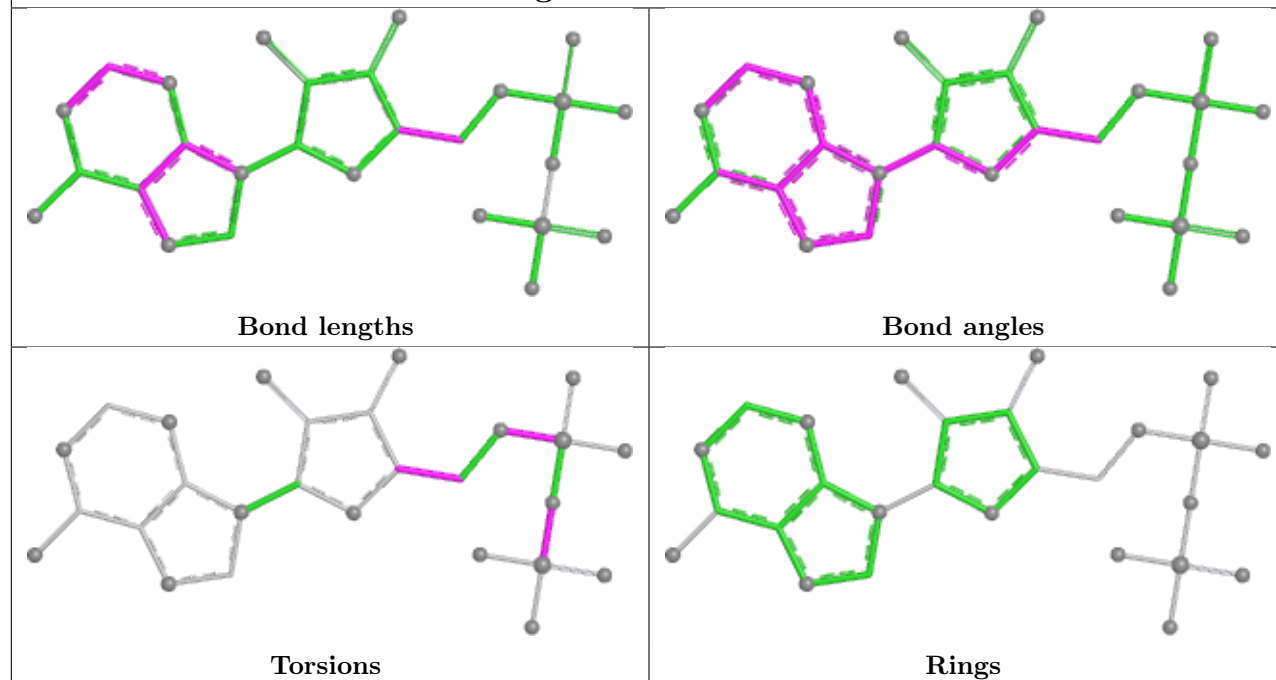
Ligand ADP e 602



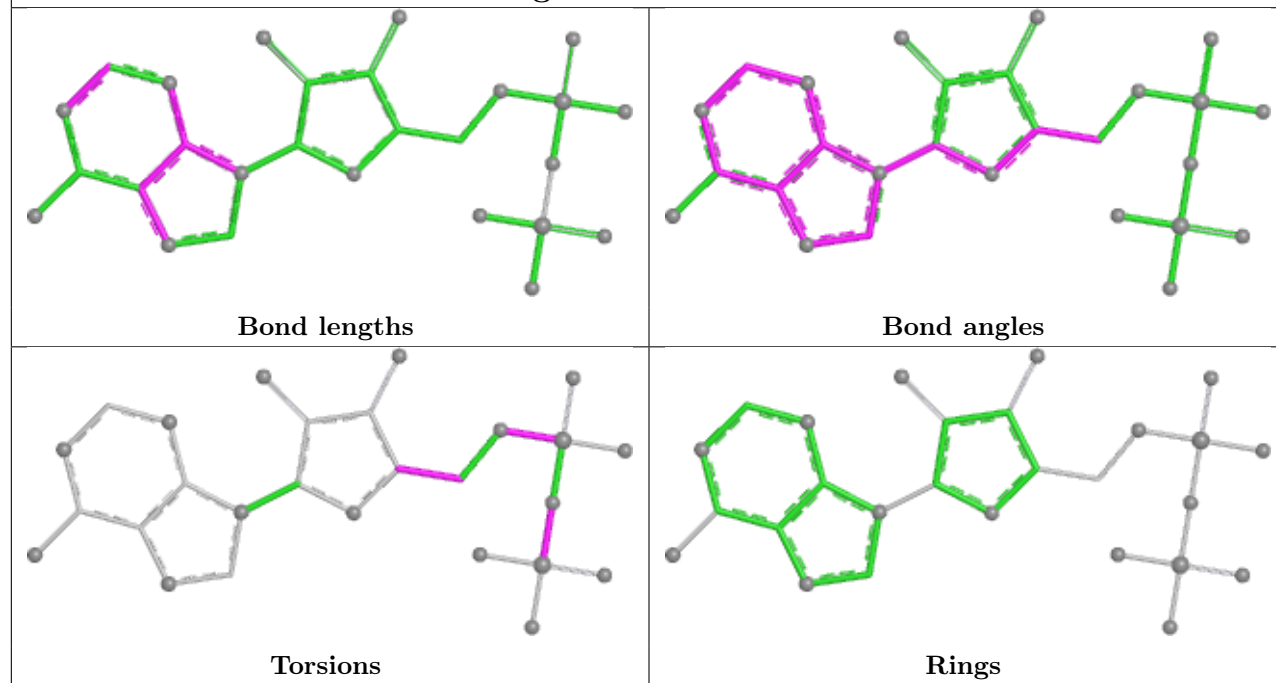
Ligand ADP b 602

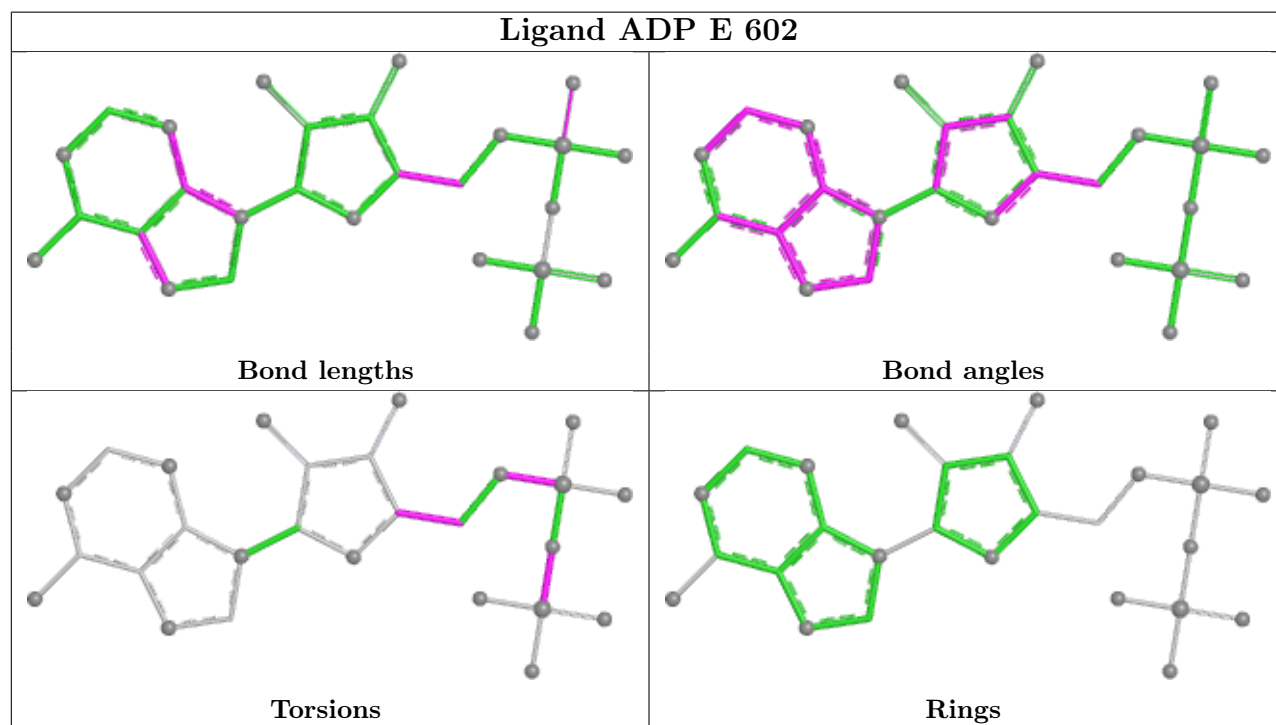
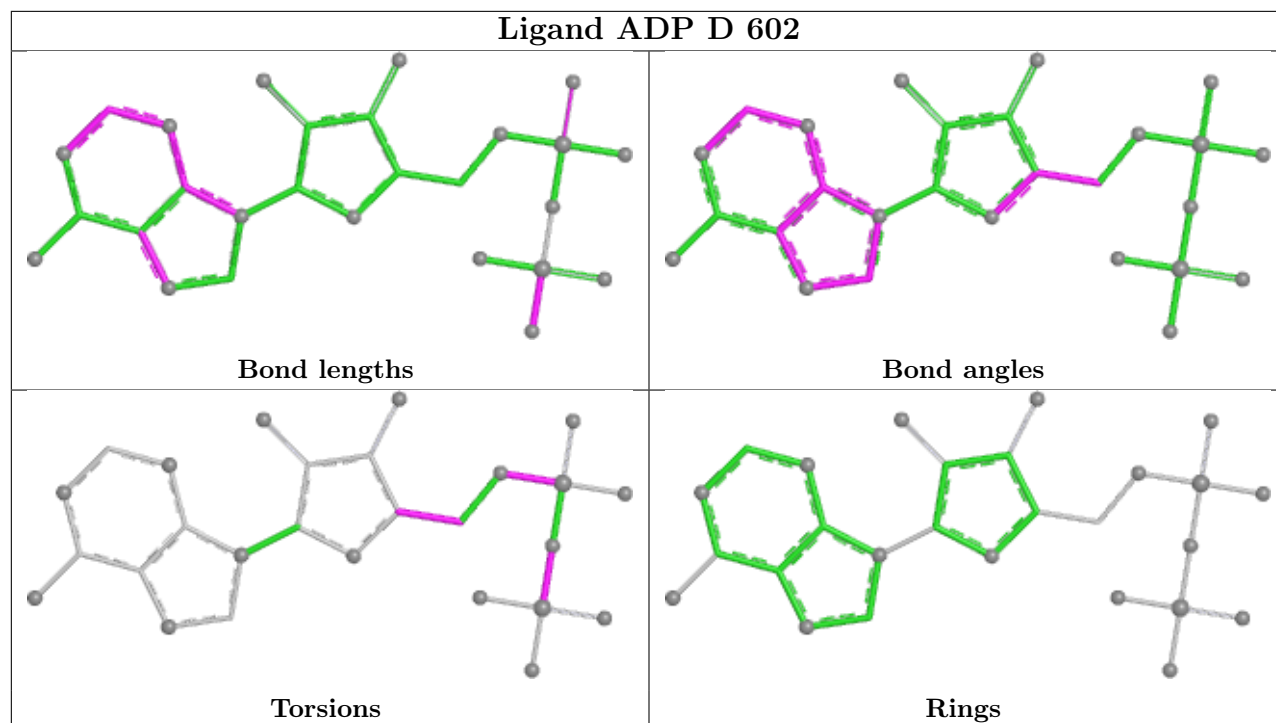


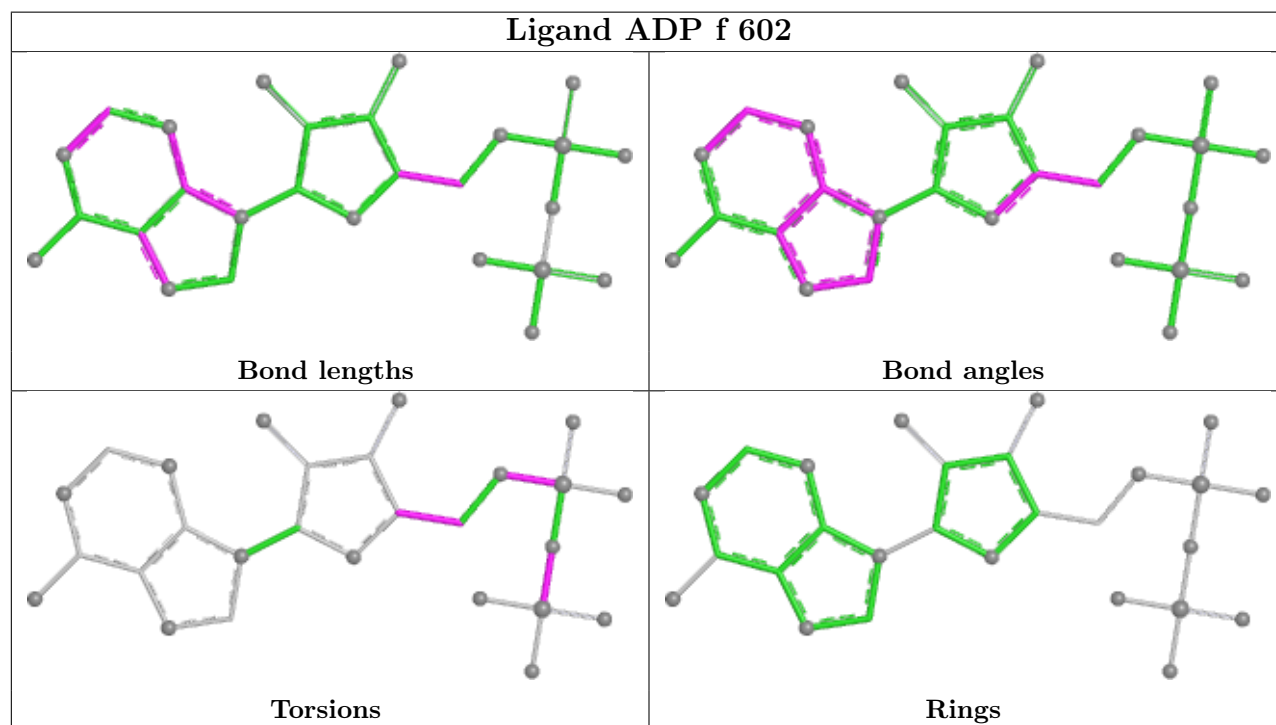
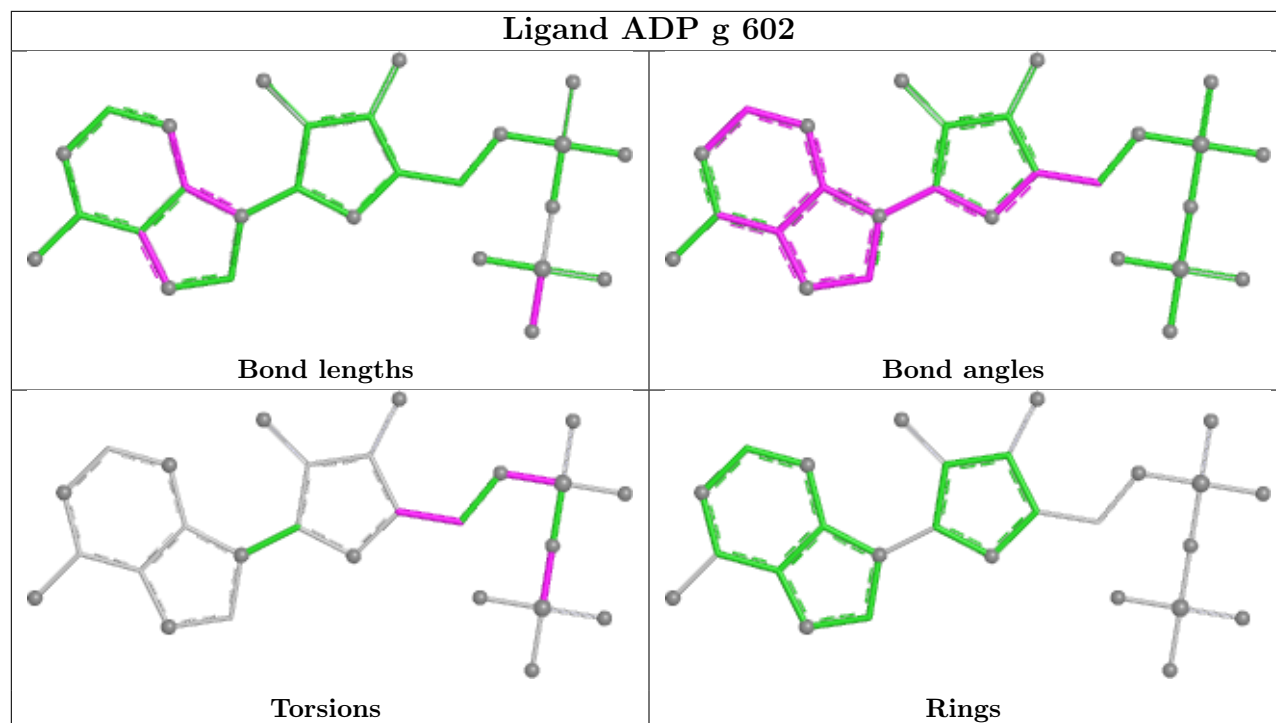
Ligand ADP c 602

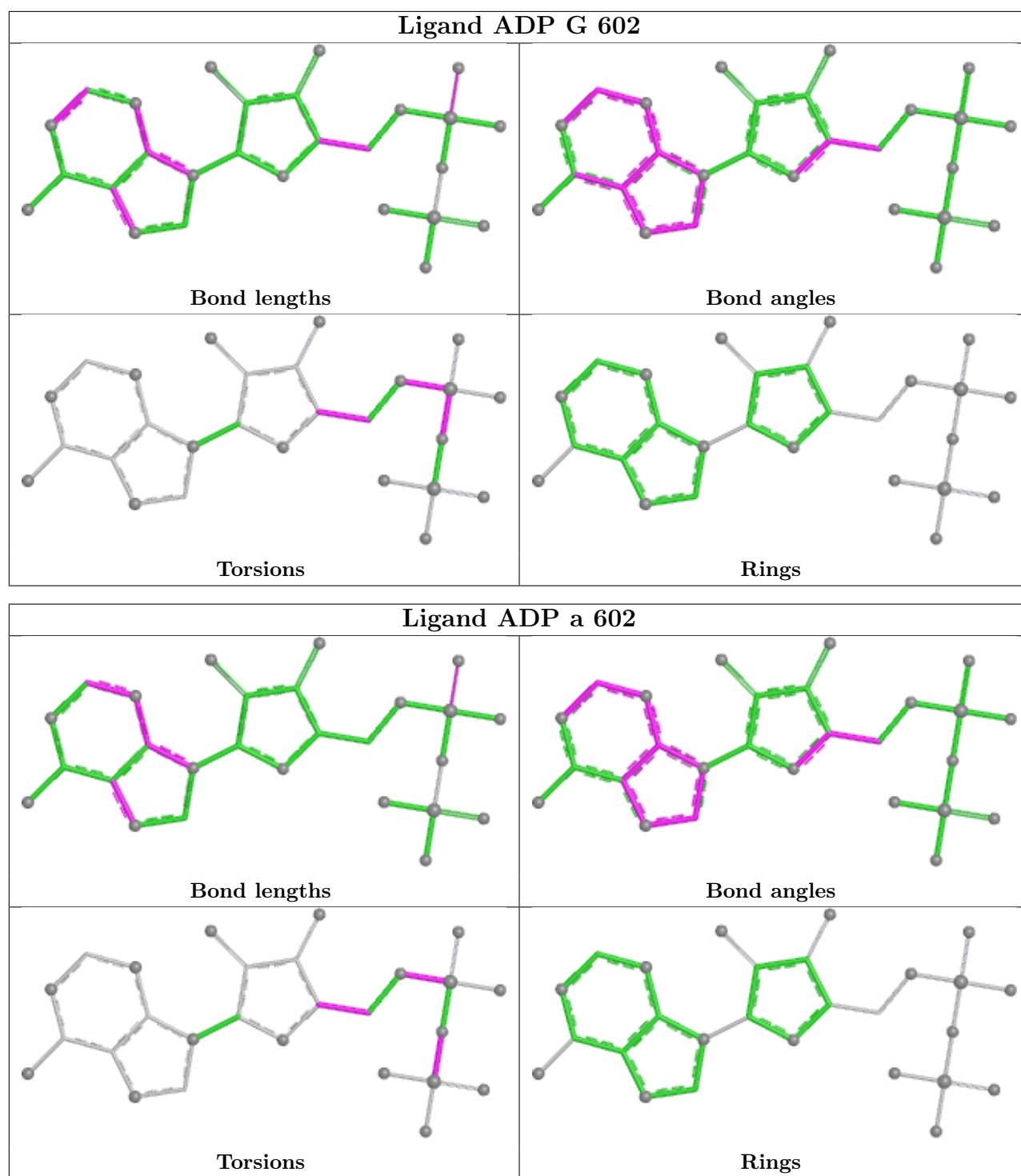


Ligand ADP d 602









5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	527/543 (97%)	-0.27	5 (0%) 81 74	16, 51, 95, 147	0
1	B	527/543 (97%)	-0.24	6 (1%) 78 70	15, 52, 101, 146	0
1	C	526/543 (96%)	-0.30	6 (1%) 78 70	14, 50, 101, 140	0
1	D	526/543 (96%)	-0.17	5 (0%) 79 72	14, 55, 120, 154	0
1	E	526/543 (96%)	-0.11	10 (1%) 66 57	9, 51, 127, 164	0
1	F	529/543 (97%)	-0.16	4 (0%) 82 75	17, 58, 108, 159	0
1	G	525/543 (96%)	-0.17	8 (1%) 72 63	19, 57, 106, 140	0
1	H	526/543 (96%)	-0.08	7 (1%) 75 66	26, 70, 120, 163	0
1	I	525/543 (96%)	-0.08	3 (0%) 85 80	24, 67, 121, 151	0
1	J	525/543 (96%)	-0.15	3 (0%) 85 80	14, 55, 110, 163	0
1	K	525/543 (96%)	-0.01	13 (2%) 58 48	16, 63, 120, 157	0
1	L	526/543 (96%)	-0.01	11 (2%) 63 54	23, 62, 115, 154	0
1	M	525/543 (96%)	1.04	125 (23%) 2 1	25, 95, 150, 167	0
1	N	526/543 (96%)	-0.00	9 (1%) 69 60	25, 70, 124, 167	0
1	a	527/543 (97%)	0.21	22 (4%) 40 32	18, 71, 128, 157	0
1	b	526/543 (96%)	0.15	37 (7%) 22 16	18, 66, 121, 163	0
1	c	527/543 (97%)	0.14	14 (2%) 56 46	23, 72, 134, 166	0
1	d	527/543 (97%)	0.23	7 (1%) 75 66	29, 77, 118, 146	0
1	e	526/543 (96%)	0.33	8 (1%) 72 63	42, 81, 116, 155	0
1	f	527/543 (97%)	0.44	11 (2%) 63 54	45, 88, 123, 149	0
1	g	526/543 (96%)	0.28	10 (1%) 66 57	27, 88, 136, 163	0
1	h	525/543 (96%)	-0.09	6 (1%) 78 70	24, 61, 112, 150	0
1	i	525/543 (96%)	0.04	8 (1%) 72 63	28, 76, 125, 160	0
1	j	525/543 (96%)	0.27	16 (3%) 52 42	32, 79, 125, 153	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	k	525/543 (96%)	0.43	12 (2%) 61 51	37, 94, 135, 158	0
1	l	525/543 (96%)	0.71	44 (8%) 17 12	48, 106, 143, 162	0
1	m	525/543 (96%)	0.90	93 (17%) 4 3	56, 104, 146, 174	0
1	n	525/543 (96%)	0.15	10 (1%) 66 57	37, 79, 130, 158	0
2	O	96/100 (96%)	0.74	4 (4%) 40 32	59, 109, 142, 146	0
2	P	94/100 (94%)	0.90	10 (10%) 11 8	69, 108, 142, 146	0
2	Q	96/100 (96%)	0.92	13 (13%) 7 5	60, 108, 142, 149	0
2	R	96/100 (96%)	0.76	5 (5%) 33 25	60, 99, 134, 151	0
2	S	96/100 (96%)	0.86	6 (6%) 26 19	61, 107, 140, 150	0
2	T	96/100 (96%)	0.88	3 (3%) 51 41	65, 106, 141, 154	0
2	U	96/100 (96%)	0.73	8 (8%) 17 12	55, 107, 142, 148	0
2	o	96/100 (96%)	0.76	5 (5%) 33 25	86, 116, 152, 164	0
2	p	96/100 (96%)	0.93	9 (9%) 14 10	80, 112, 146, 150	0
2	q	96/100 (96%)	0.52	2 (2%) 63 54	45, 101, 141, 157	0
2	r	96/100 (96%)	0.92	11 (11%) 9 7	60, 109, 141, 150	0
2	s	96/100 (96%)	1.03	9 (9%) 14 10	73, 114, 143, 150	0
2	t	96/100 (96%)	0.65	4 (4%) 40 32	82, 118, 147, 159	0
2	u	96/100 (96%)	0.53	3 (3%) 51 41	83, 122, 153, 167	0
All	All	16067/16604 (96%)	0.18	605 (3%) 44 35	9, 76, 133, 174	0

The worst 5 of 605 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	294	VAL	13.5
1	M	291	ILE	11.3
1	M	295	THR	7.9
1	M	273	ALA	7.2
1	M	219	ILE	7.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DMS	k	601	4/4	0.80	0.27	89,96,103,115	0
5	DMS	l	601	4/4	0.83	0.22	63,95,106,125	0
5	DMS	j	601	4/4	0.84	0.15	82,83,101,117	0
5	DMS	L	601	4/4	0.85	0.17	39,58,61,94	0
3	MG	d	601	1/1	0.86	0.12	68,68,68,68	0
5	DMS	n	701	4/4	0.86	0.20	69,85,87,99	0
5	DMS	m	601	4/4	0.88	0.17	82,92,95,105	0
3	MG	b	601	1/1	0.89	0.12	53,53,53,53	0
5	DMS	J	601	4/4	0.89	0.14	39,53,65,90	0
5	DMS	M	601	4/4	0.91	0.10	26,29,60,79	0
5	DMS	h	601	4/4	0.91	0.13	52,58,85,96	0
5	DMS	i	601	4/4	0.91	0.10	27,32,40,87	0
3	MG	f	601	1/1	0.91	0.07	70,70,70,70	0
3	MG	g	601	1/1	0.92	0.12	66,66,66,66	0
4	ADP	e	602	27/27	0.92	0.10	48,78,103,108	0
4	ADP	f	602	27/27	0.93	0.10	47,93,109,116	0
4	ADP	d	602	27/27	0.93	0.09	45,72,87,93	0
5	DMS	K	601	4/4	0.93	0.10	43,44,76,91	0
3	MG	e	601	1/1	0.93	0.11	62,62,62,62	0
3	MG	E	601	1/1	0.94	0.06	20,20,20,20	0
4	ADP	c	602	27/27	0.95	0.09	24,67,80,102	0
3	MG	A	601	1/1	0.95	0.07	27,27,27,27	0
3	MG	F	601	1/1	0.95	0.06	25,25,25,25	0
3	MG	C	601	1/1	0.95	0.05	28,28,28,28	0
4	ADP	g	602	27/27	0.95	0.09	56,84,98,103	0
3	MG	c	601	1/1	0.95	0.11	51,51,51,51	0
4	ADP	D	602	27/27	0.95	0.08	1,38,64,69	0
4	ADP	a	602	27/27	0.95	0.09	21,70,81,90	0
4	ADP	b	602	27/27	0.96	0.07	13,58,79,85	0
4	ADP	E	602	27/27	0.96	0.08	12,44,74,80	0
4	ADP	C	602	27/27	0.96	0.08	1,34,70,78	0
5	DMS	H	601	4/4	0.96	0.11	24,28,74,96	0

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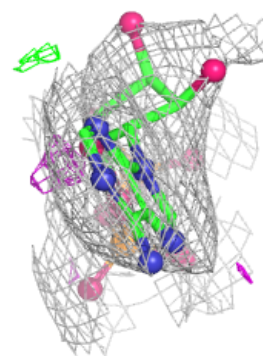
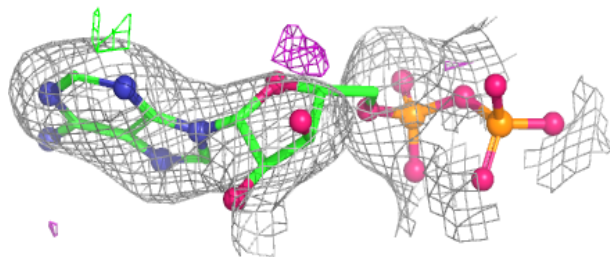
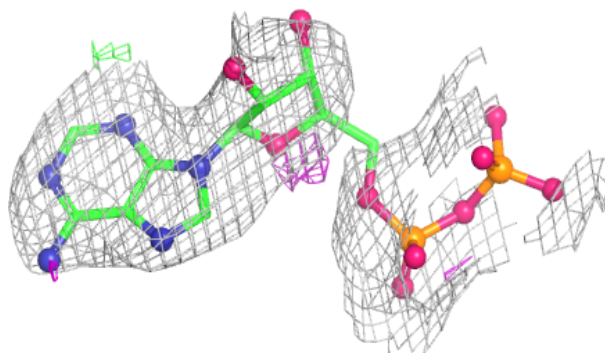
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	DMS	N	701	4/4	0.96	0.12	53,57,64,90	0
5	DMS	I	601	4/4	0.96	0.07	37,58,66,93	0
4	ADP	A	602	27/27	0.97	0.07	1,47,68,77	0
4	ADP	F	602	27/27	0.97	0.07	23,51,75,88	0
4	ADP	G	602	27/27	0.97	0.07	1,61,76,85	0
4	ADP	B	602	27/27	0.97	0.08	18,54,75,80	0
3	MG	B	601	1/1	0.97	0.13	44,44,44,44	0
3	MG	G	601	1/1	0.97	0.06	29,29,29,29	0
3	MG	D	601	1/1	0.98	0.10	29,29,29,29	0
3	MG	a	601	1/1	0.98	0.06	54,54,54,54	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.

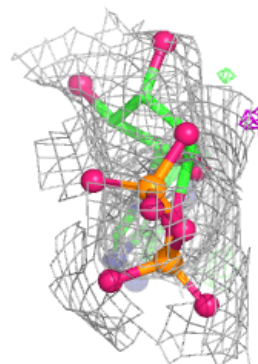
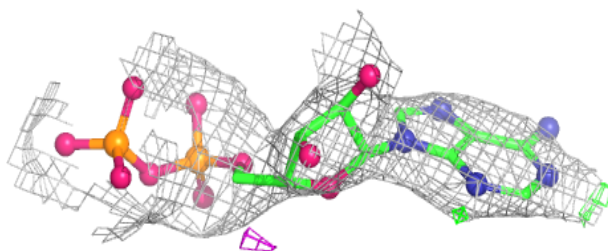
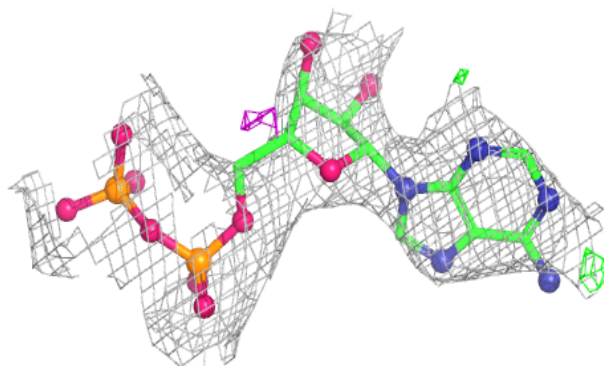
Electron density around ADP e 602:

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

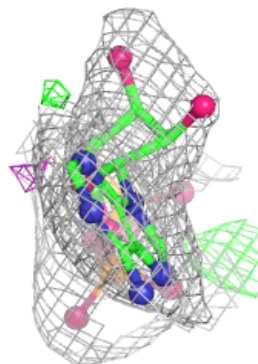
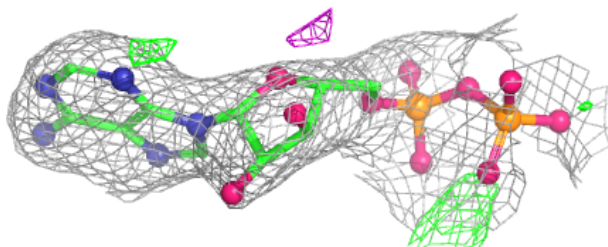
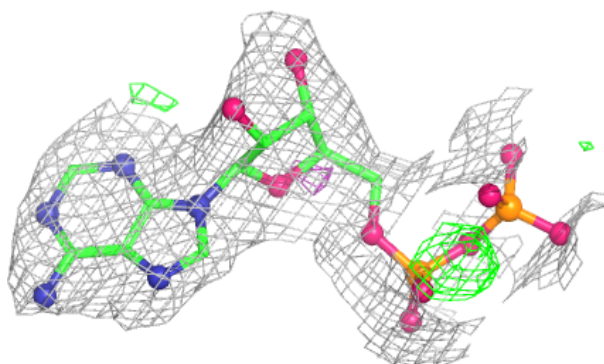


Electron density around ADP f 602:

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

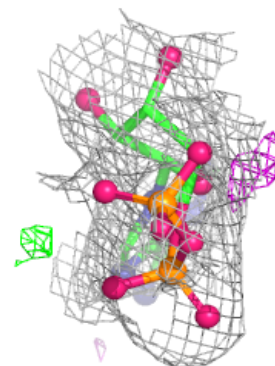
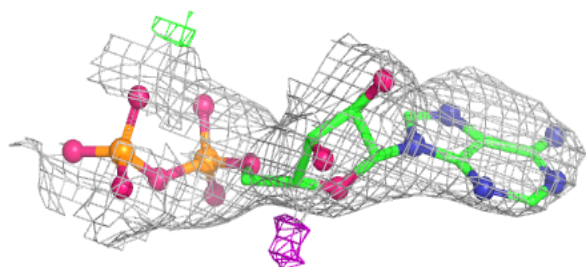
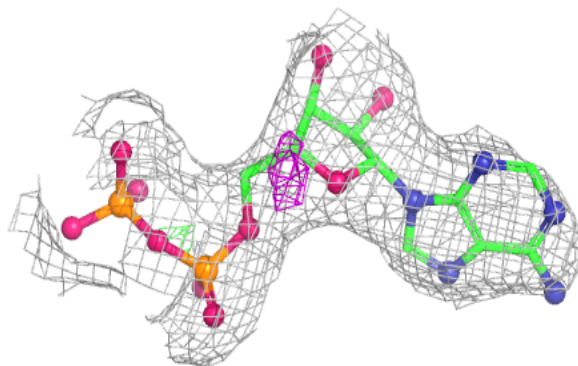
**Electron density around ADP d 602:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

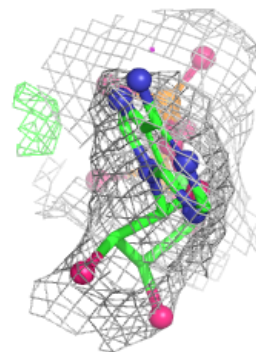
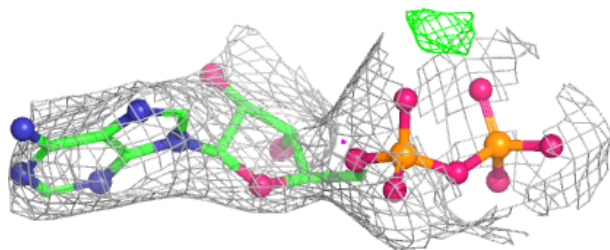
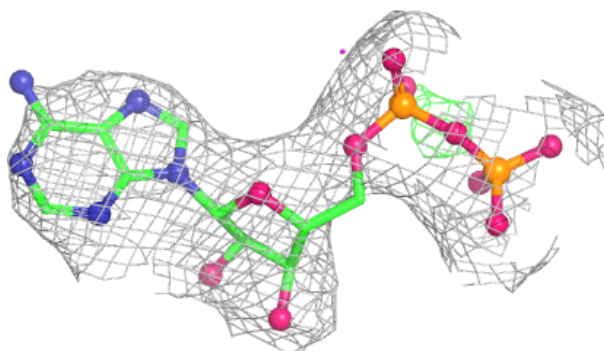


Electron density around ADP c 602:

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and green (positive)

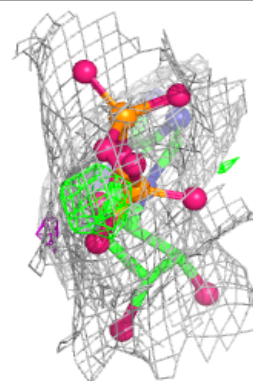
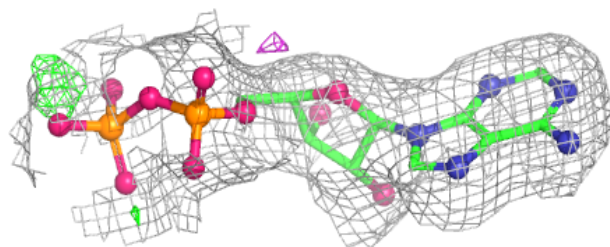
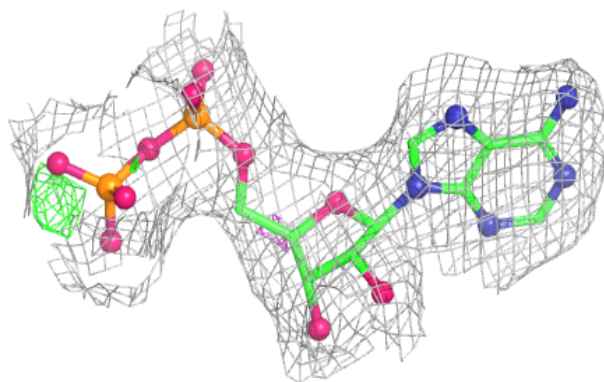
**Electron density around ADP g 602:**

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

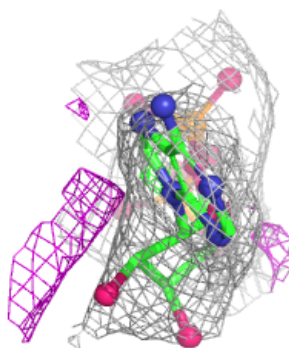
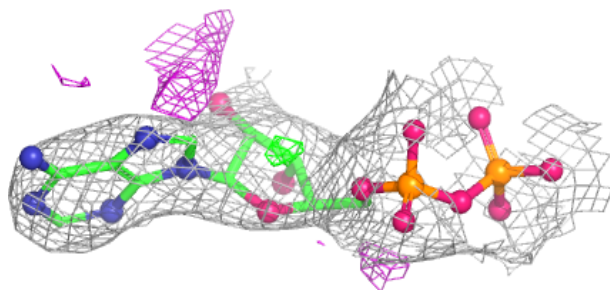
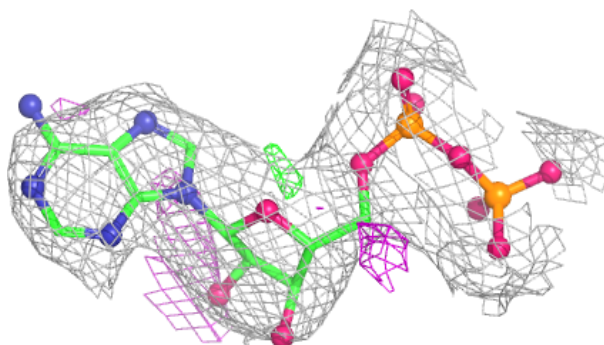


Electron density around ADP D 602:

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and green (positive)

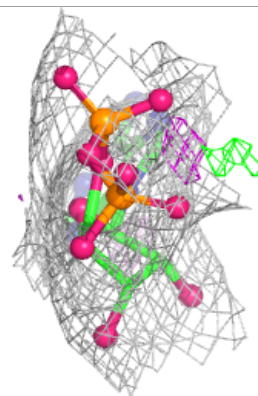
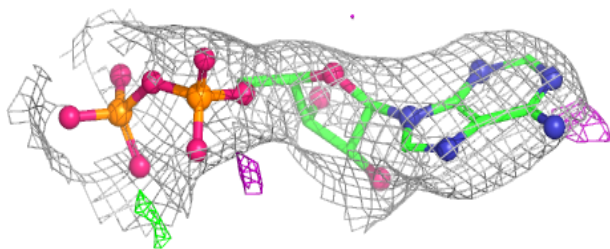
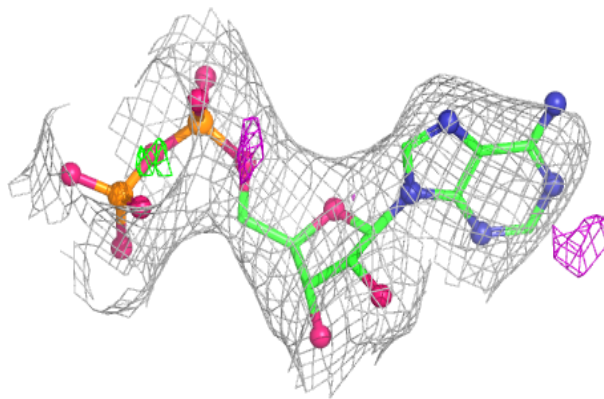
**Electron density around ADP a 602:**

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

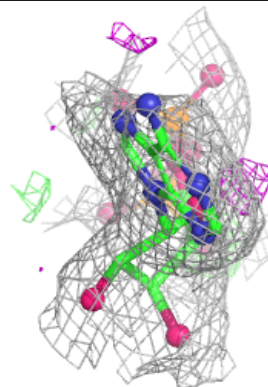
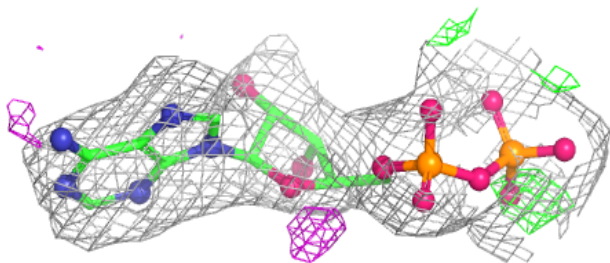
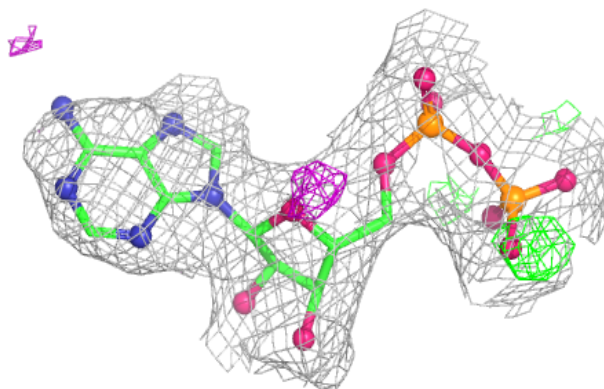


Electron density around ADP b 602:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

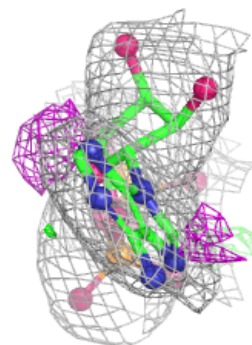
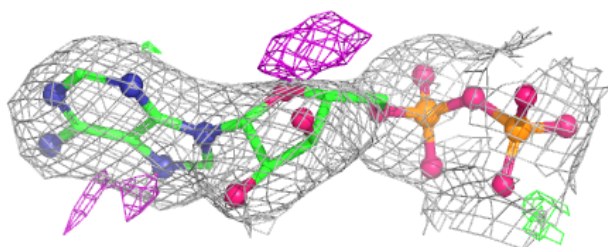
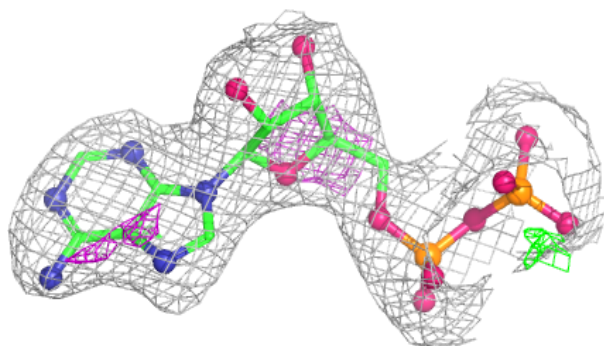
**Electron density around ADP E 602:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

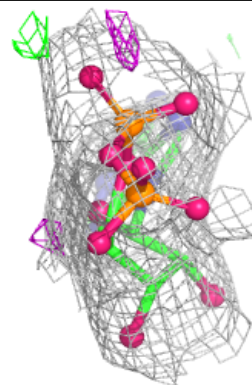
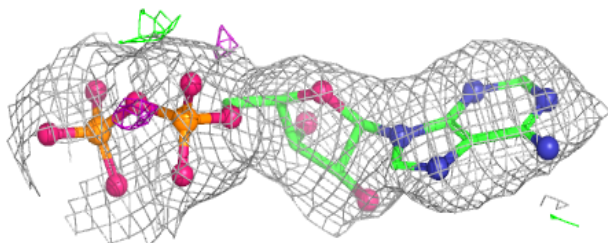
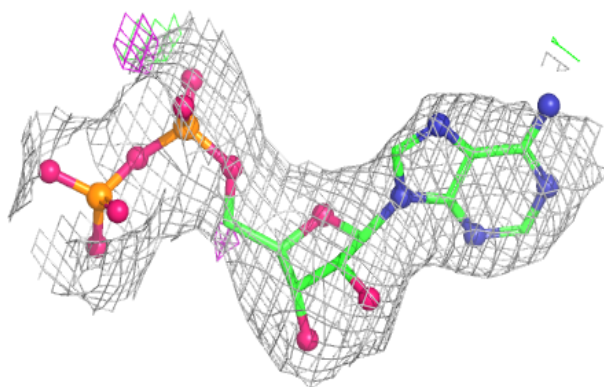


Electron density around ADP C 602:

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

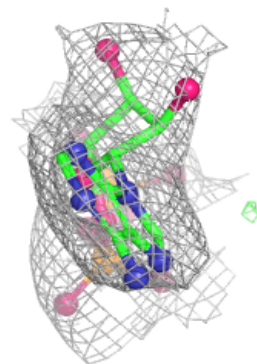
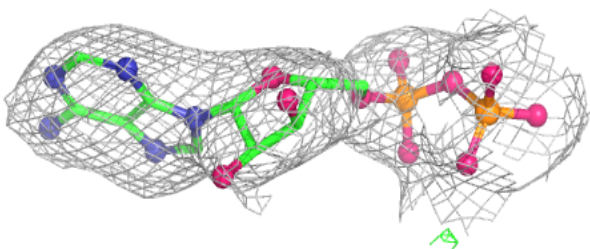
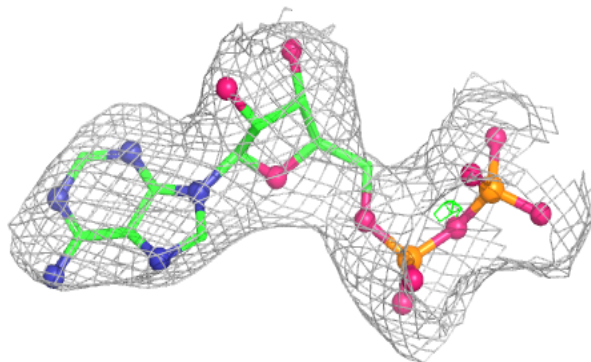
**Electron density around ADP A 602:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

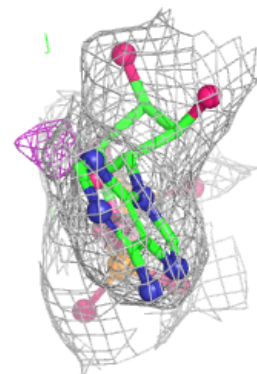
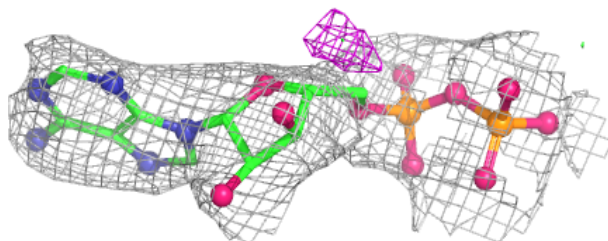
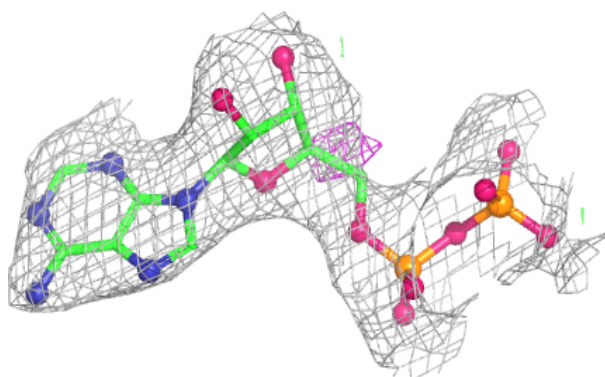


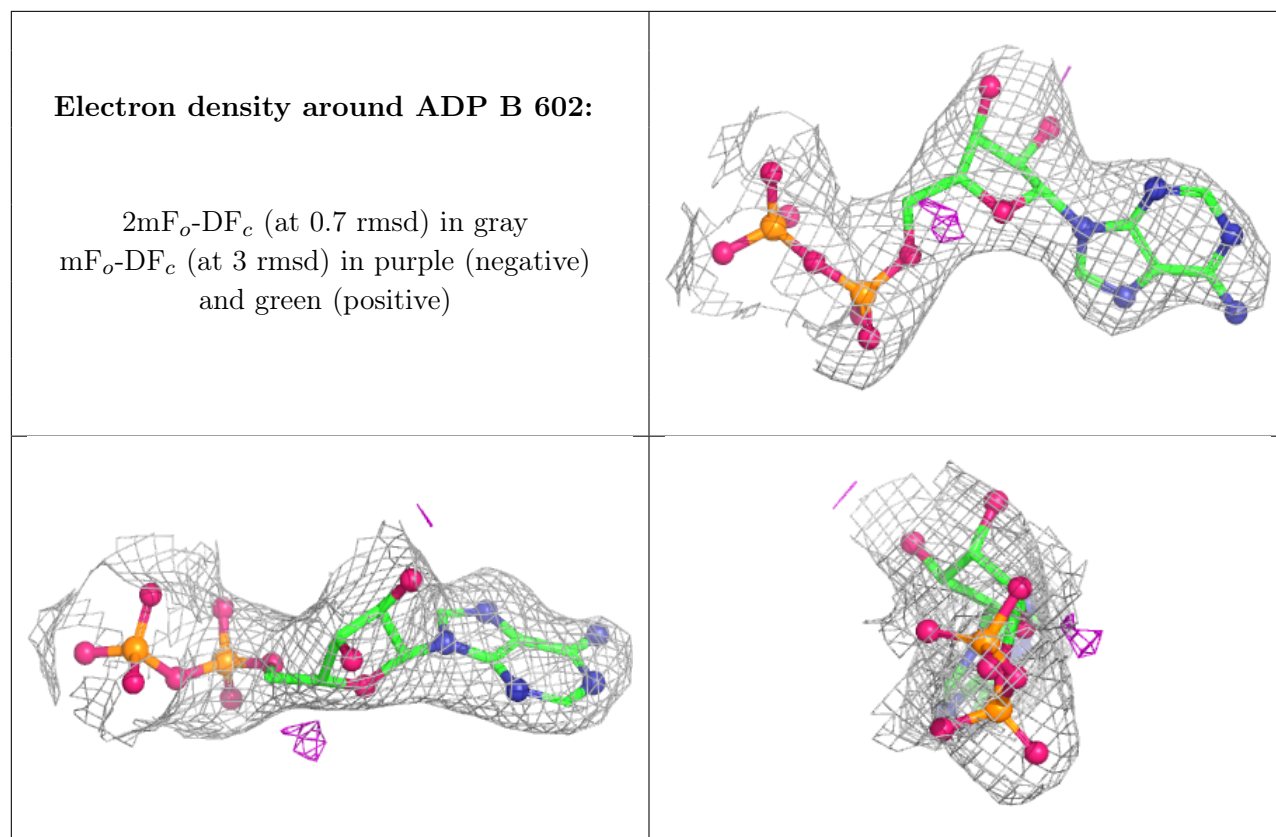
Electron density around ADP F 602:

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

**Electron density around ADP G 602:**

$2mF_o - DF_c$ (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.