wwPDB X-ray Structure Validation Summary Report (i)

Mar 13, 2024 – 08:34 AM EDT

PDB ID	:	4V4O
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 (i) symbol.

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

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

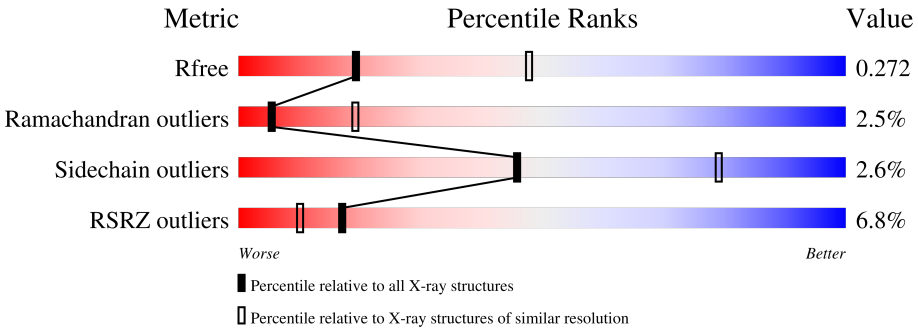
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 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}	130704	3140 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (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 <=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	93%
1	B	543	93%
1	C	543	92% 5%
1	D	543	92%
1	E	543	90% 6%
1	F	543	93%

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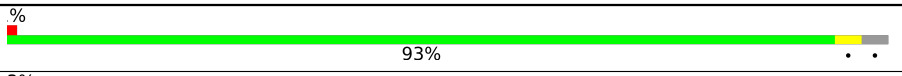
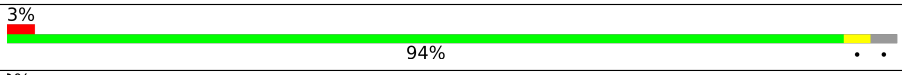
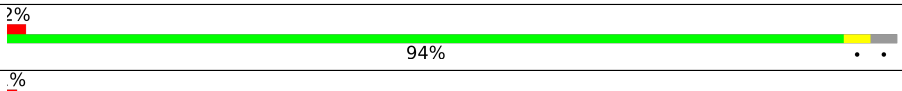
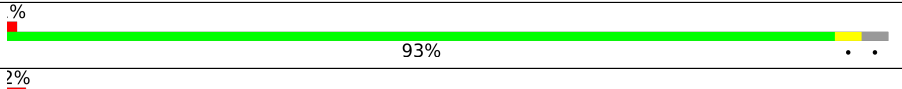
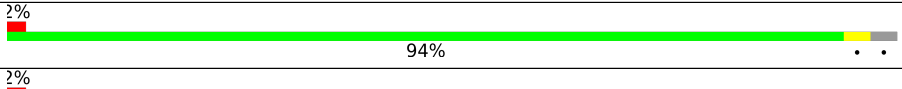
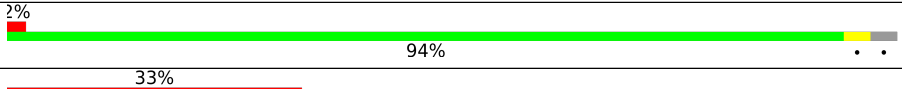
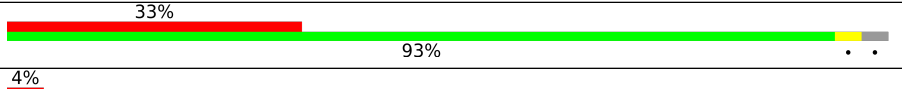
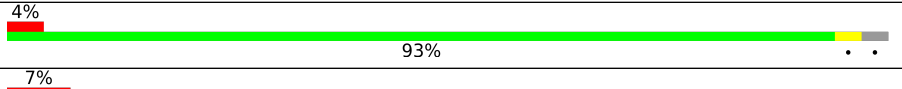
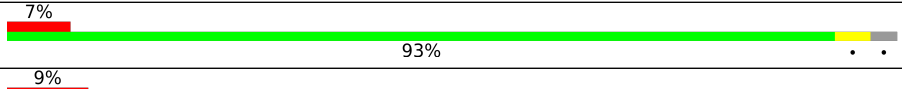
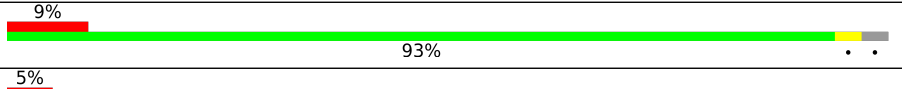
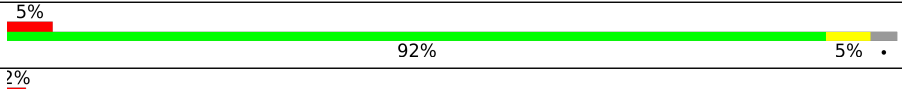
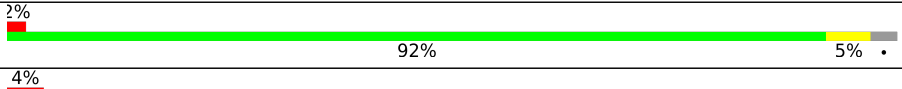
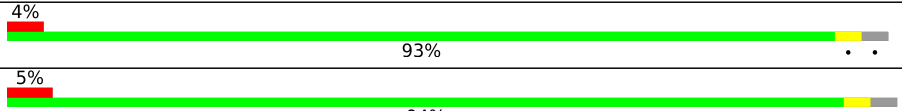
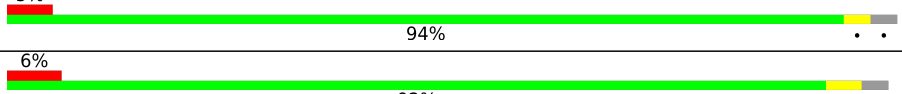
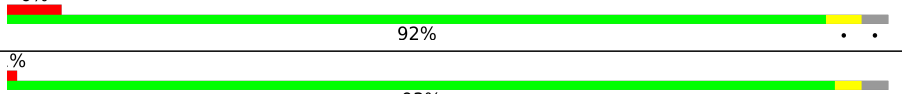
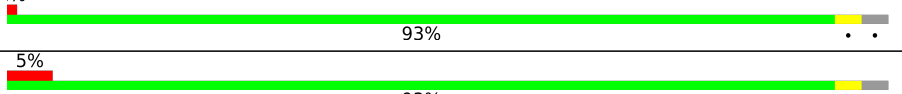
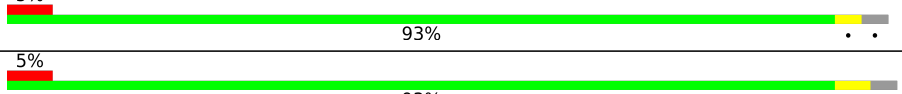
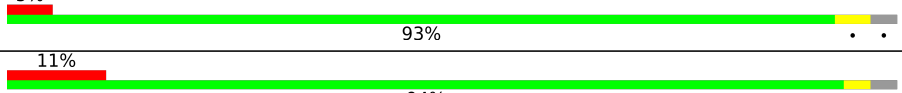
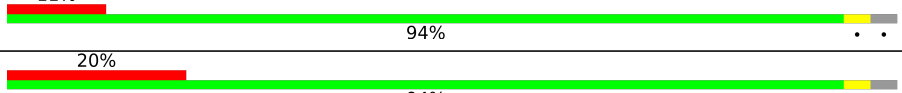
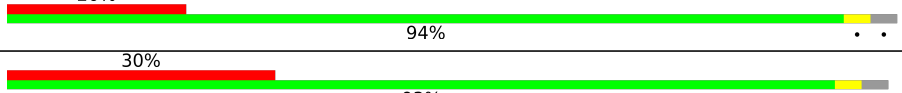
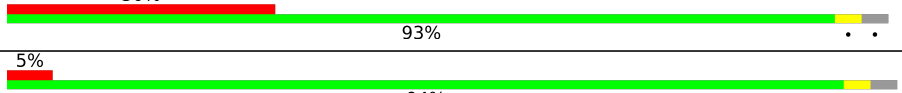
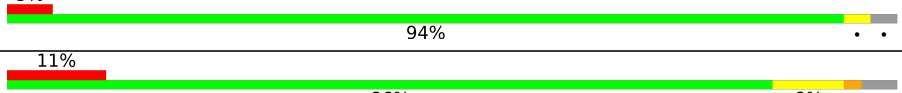
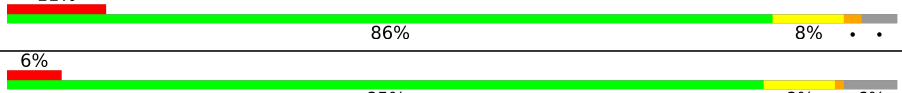
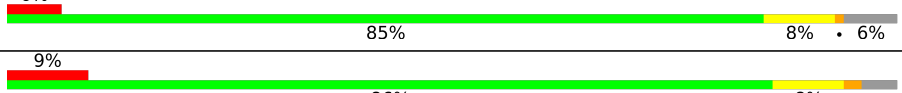
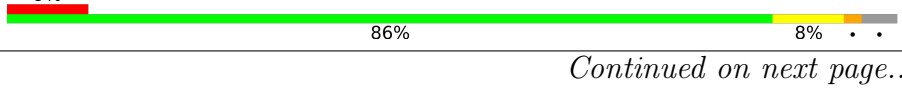
Mol	Chain	Length	Quality of chain
1	G	543	
1	H	543	
1	I	543	
1	J	543	
1	K	543	
1	L	543	
1	M	543	
1	N	543	
1	a	543	
1	b	543	
1	c	543	
1	d	543	
1	e	543	
1	f	543	
1	g	543	
1	h	543	
1	i	543	
1	j	543	
1	k	543	
1	l	543	
1	m	543	
1	n	543	
2	O	100	
2	P	100	
2	Q	100	

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Mol	Chain	Length	Quality of chain
2	R	100	6% 85% 11%
2	S	100	14% 87% 9%
2	T	100	11% 86% 9%
2	U	100	10% 86% 10%
2	o	100	28% 88% 8%
2	p	100	14% 86% 10%
2	q	100	5% 79% 16%
2	r	100	10% 87% 9%
2	s	100	14% 88% 8%
2	t	100	16% 85% 11%
2	u	100	17% 84% 11%

2 Entry composition (i)

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 739	C 470	N 126	O 143	0	0	0
2	p	96	Total 739	C 470	N 126	O 143	0	0	0
2	q	96	Total 739	C 470	N 126	O 143	0	0	0
2	r	96	Total 739	C 470	N 126	O 143	0	0	0
2	s	96	Total 739	C 470	N 126	O 143	0	0	0
2	t	96	Total 739	C 470	N 126	O 143	0	0	0
2	u	96	Total 739	C 470	N 126	O 143	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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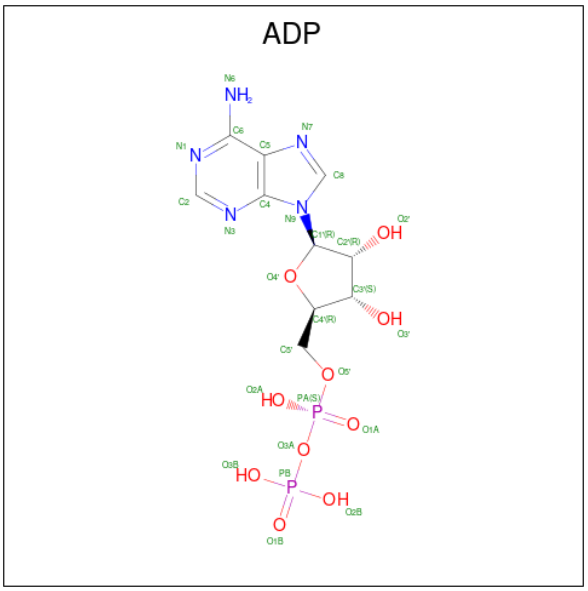
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	f	1	Total Mg 1 1	0	0
3	g	1	Total Mg 1 1	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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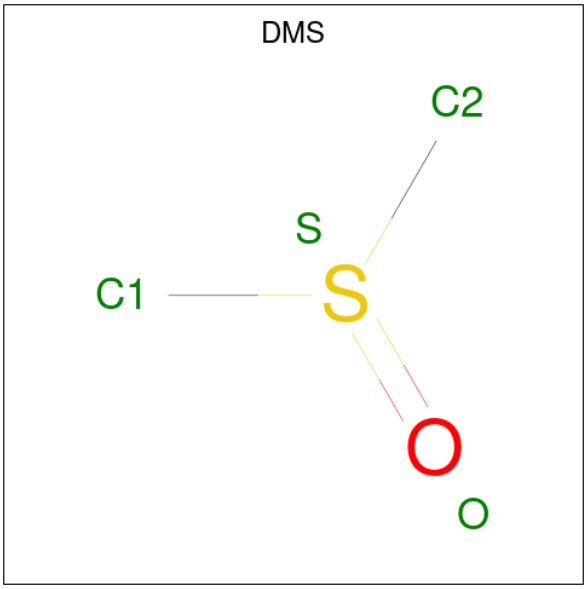
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	c	1	Total C N O P 27 10 5 10 2	0	0
4	d	1	Total C N O P 27 10 5 10 2	0	0
4	e	1	Total C N O P 27 10 5 10 2	0	0
4	f	1	Total C N O P 27 10 5 10 2	0	0
4	g	1	Total C N O P 27 10 5 10 2	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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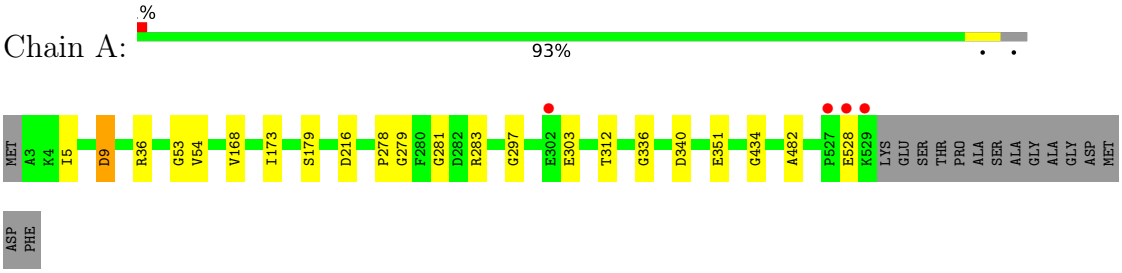
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	N	1	Total	C	O	S	0	0
			4	2	1	1		
5	h	1	Total	C	O	S	0	0
			4	2	1	1		
5	i	1	Total	C	O	S	0	0
			4	2	1	1		
5	j	1	Total	C	O	S	0	0
			4	2	1	1		
5	k	1	Total	C	O	S	0	0
			4	2	1	1		
5	l	1	Total	C	O	S	0	0
			4	2	1	1		
5	m	1	Total	C	O	S	0	0
			4	2	1	1		
5	n	1	Total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

3 Residue-property plots (i)

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

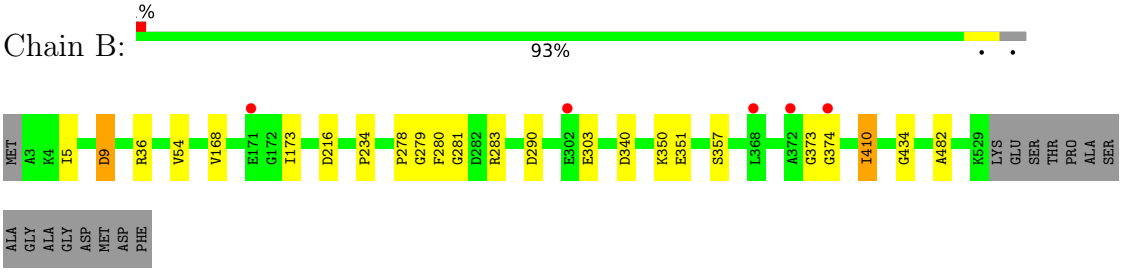
• Molecule 1: cpn60(GroEL)

Chain A:



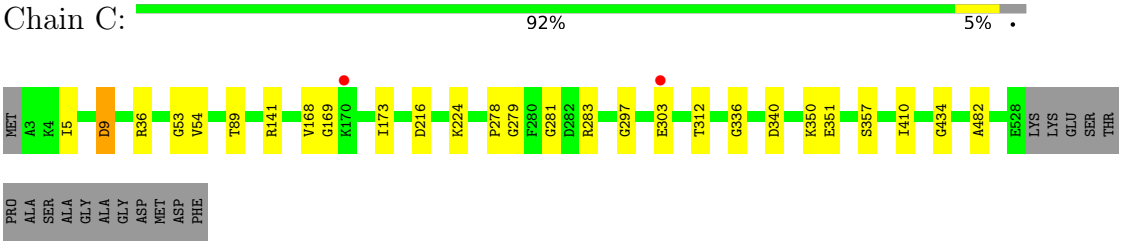
• Molecule 1: cpn60(GroEL)

Chain B:



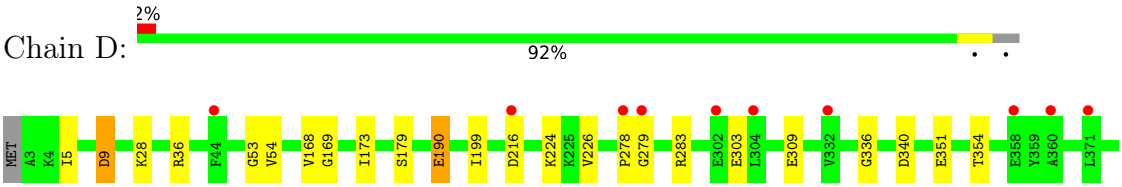
• Molecule 1: cpn60(GroEL)

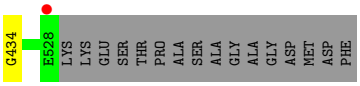
Chain C:



• Molecule 1: cpn60(GroEL)

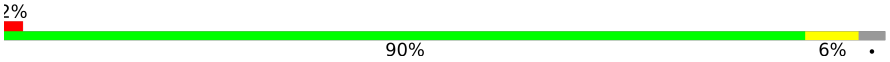
Chain D:

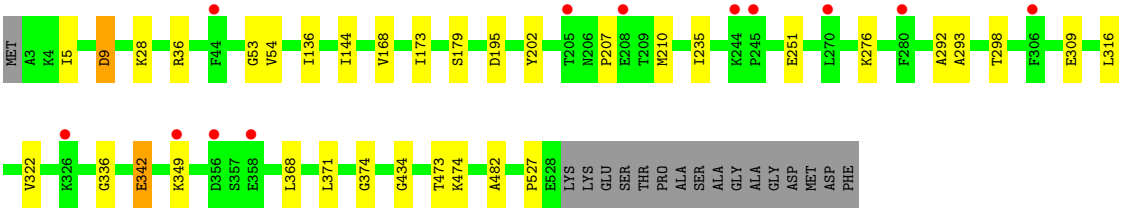




• Molecule 1: cpn60(GroEL)

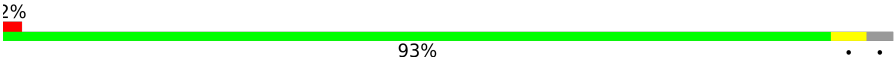
Chain E:

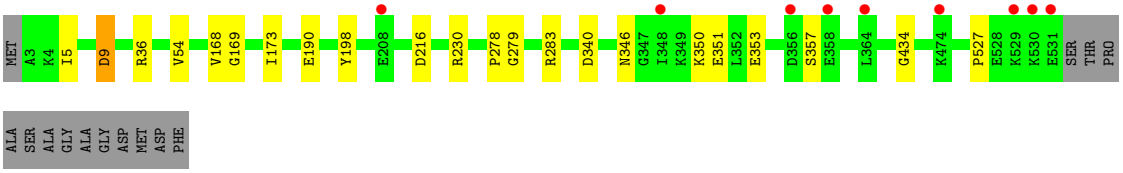




• Molecule 1: cpn60(GroEL)

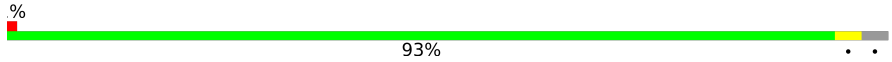
Chain F:

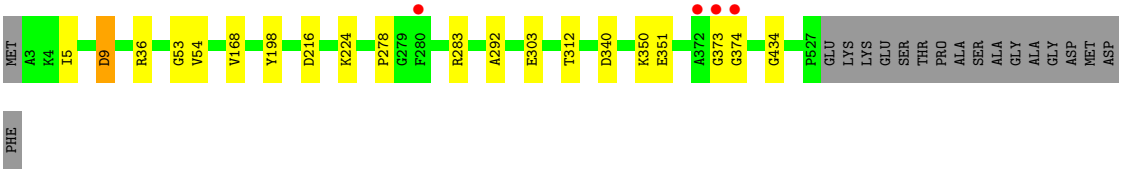




• Molecule 1: cpn60(GroEL)

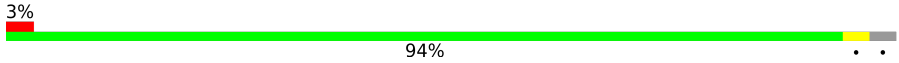
Chain G:

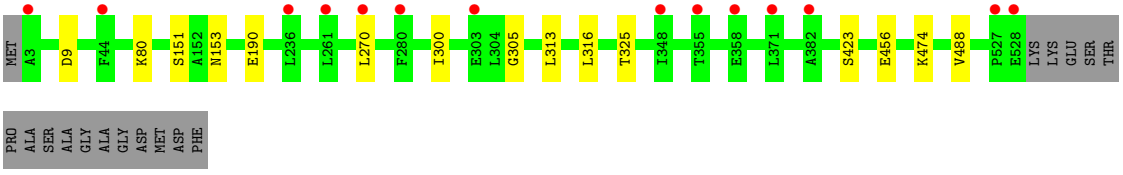




• Molecule 1: cpn60(GroEL)

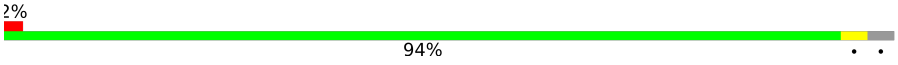
Chain H:

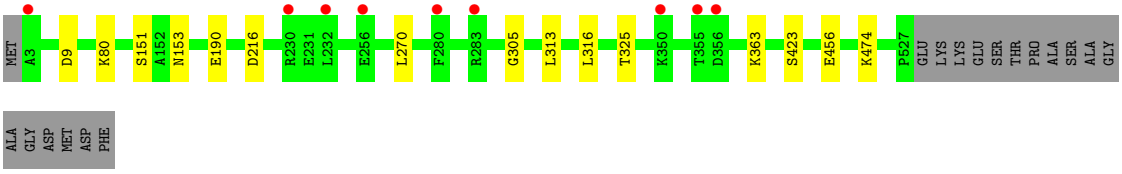




• Molecule 1: cpn60(GroEL)

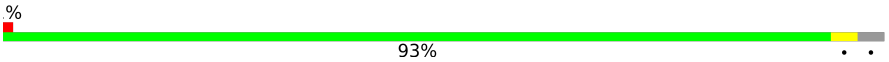
Chain I:





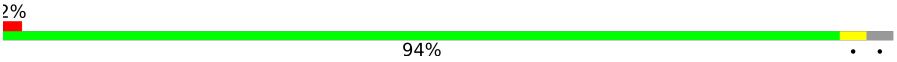
• Molecule 1: cpn60(GroEL)

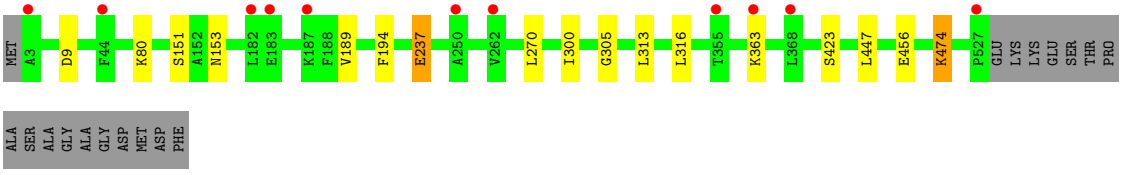
Chain J:



• Molecule 1: cpn60(GroEL)

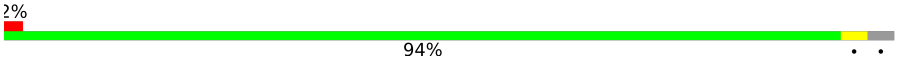
Chain K:

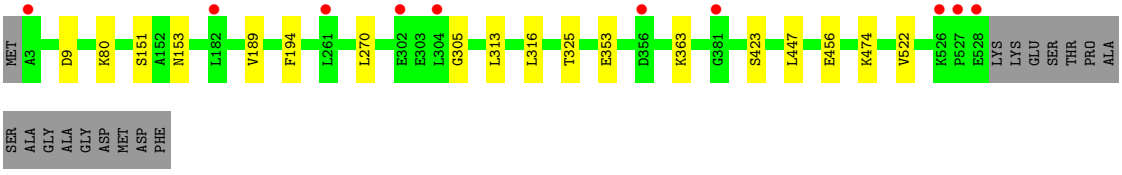




• Molecule 1: cpn60(GroEL)

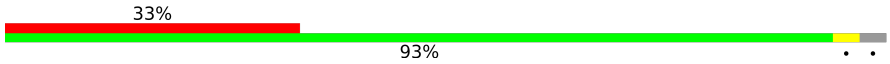
Chain L:

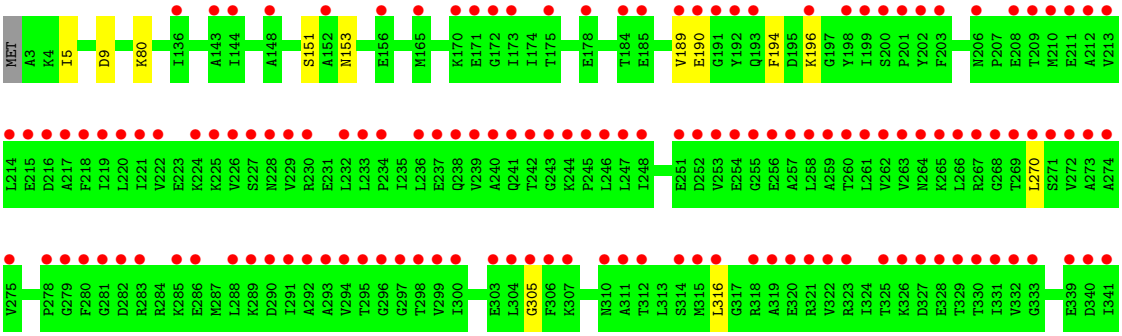


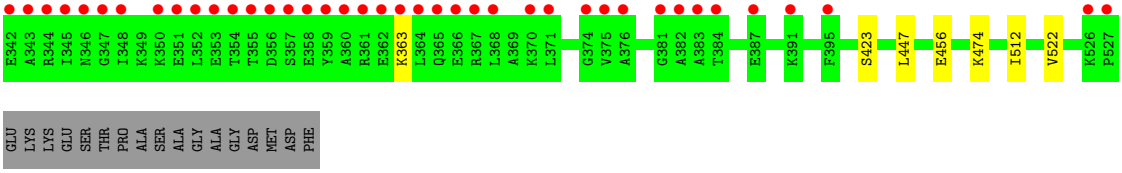


• Molecule 1: cpn60(GroEL)

Chain M:

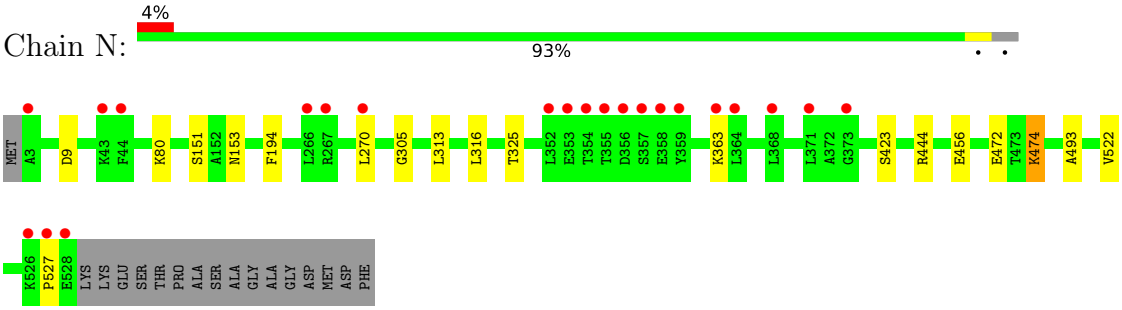






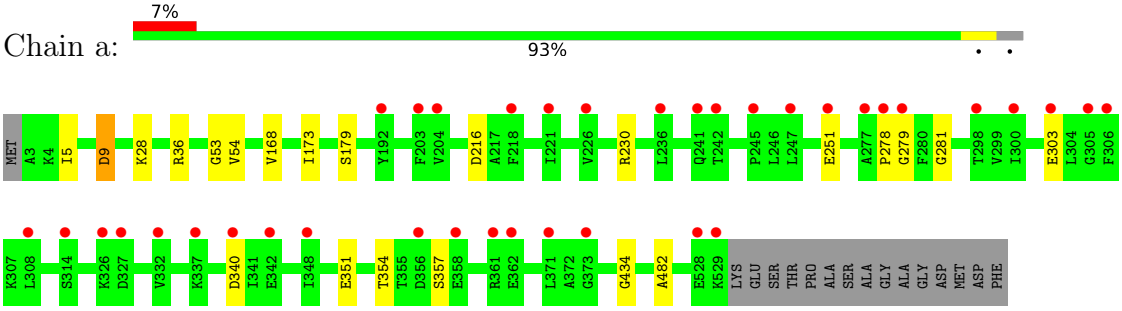
• Molecule 1: cpn60(GroEL)

Chain N:



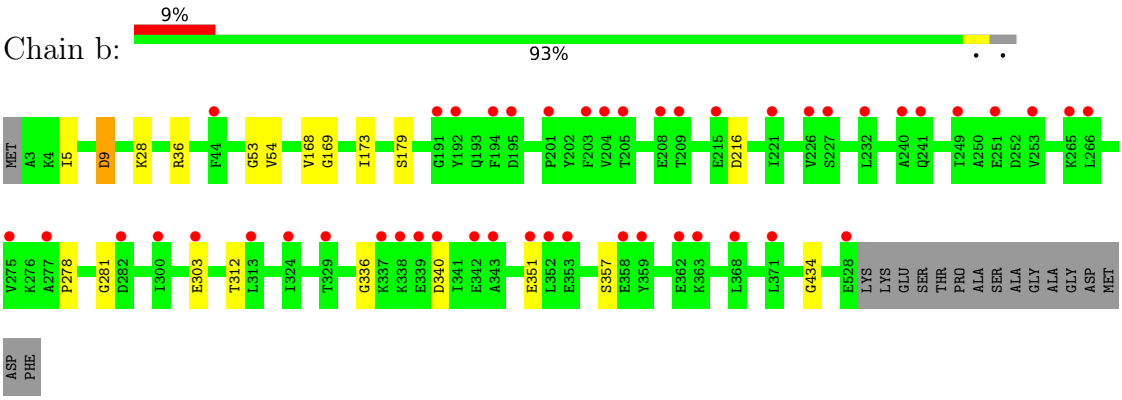
• Molecule 1: cpn60(GroEL)

Chain a:



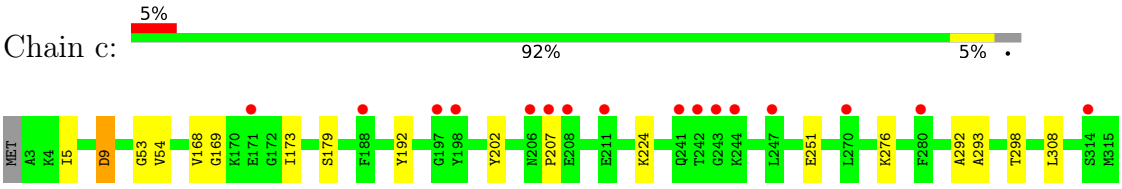
• Molecule 1: cpn60(GroEL)

Chain b:



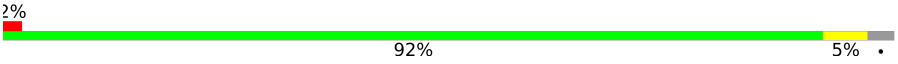
• Molecule 1: cpn60(GroEL)

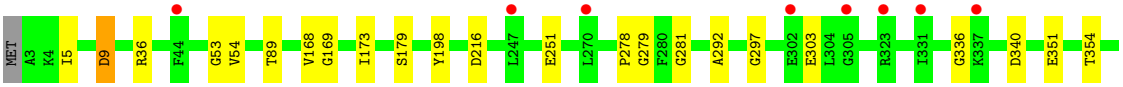
Chain c:

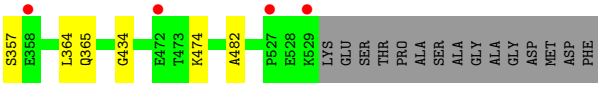


• Molecule 1: cpn60(GroEL)

Chain d:

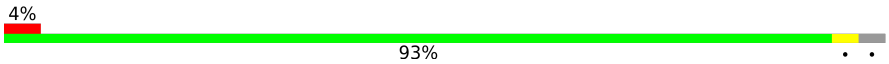


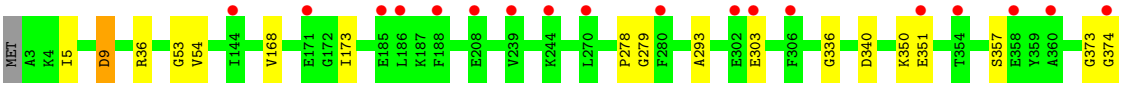


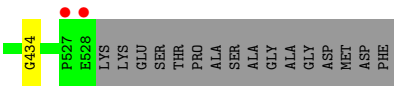


• Molecule 1: cpn60(GroEL)

Chain e:

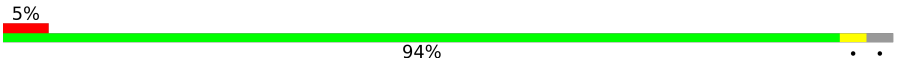


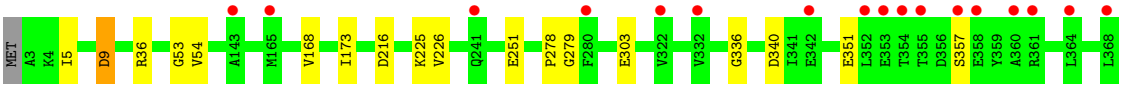


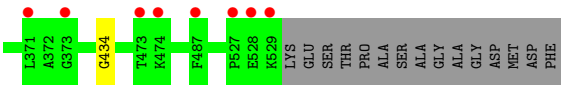


• Molecule 1: cpn60(GroEL)

Chain f:

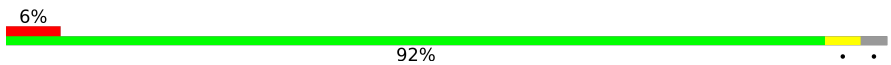


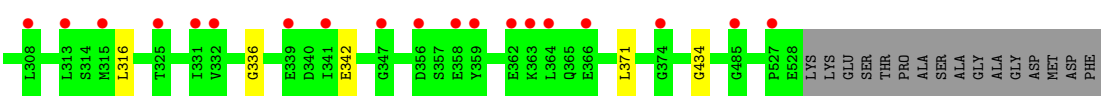




• Molecule 1: cpn60(GroEL)

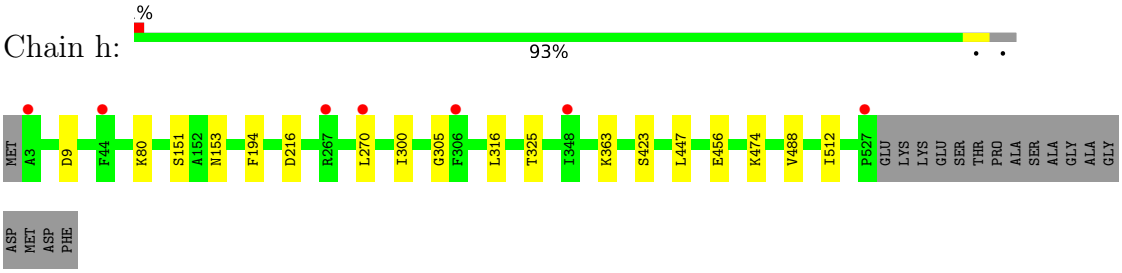
Chain g:





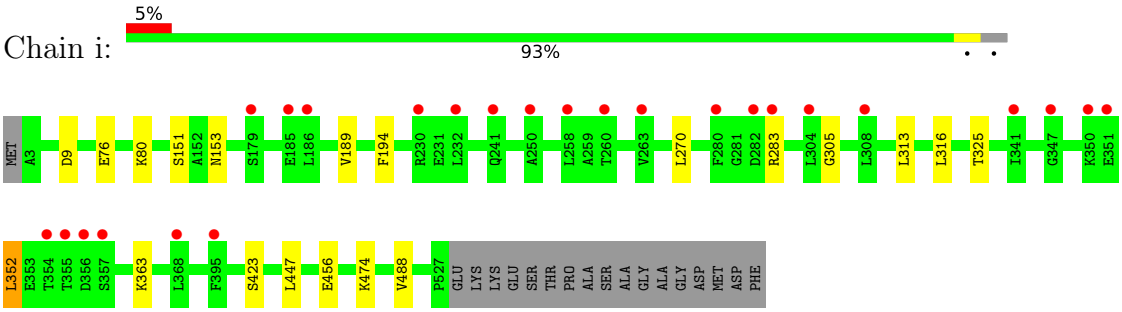
• Molecule 1: cpn60(GroEL)

Chain h:



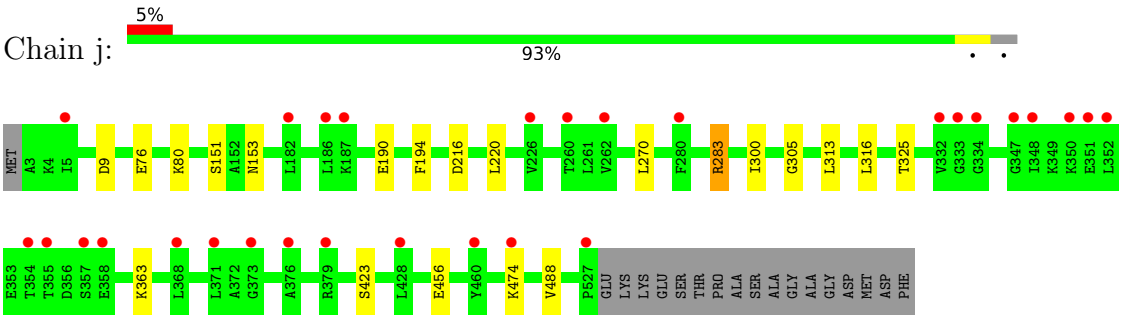
• Molecule 1: cpn60(GroEL)

Chain i:



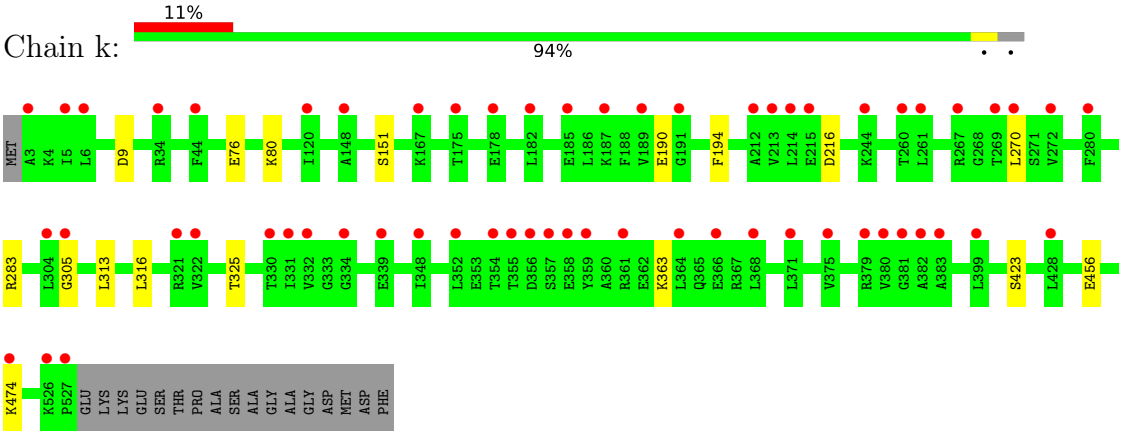
• Molecule 1: cpn60(GroEL)

Chain j:



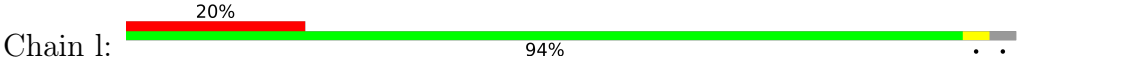
• Molecule 1: cpn60(GroEL)

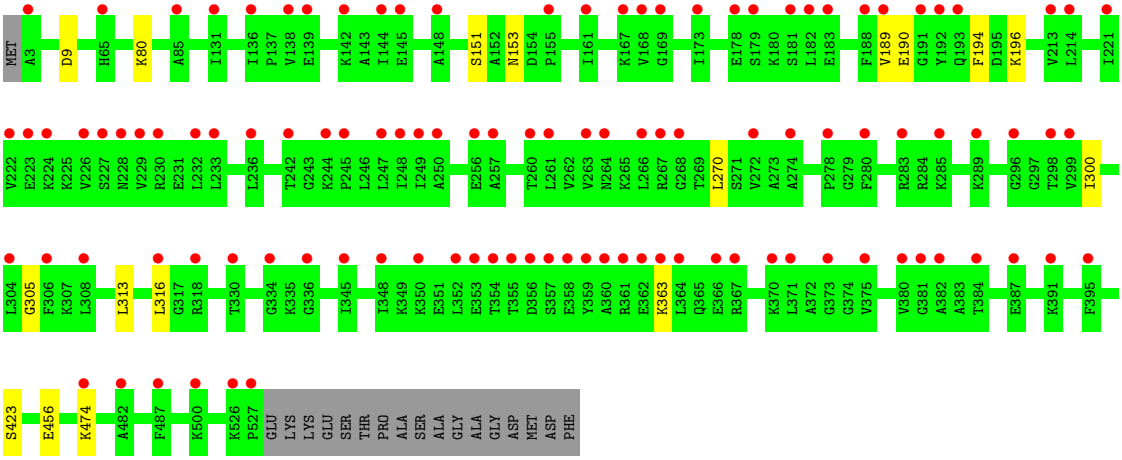
Chain k:



• Molecule 1: cpn60(GroEL)

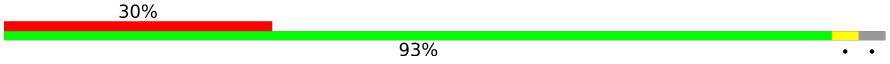
Chain l:

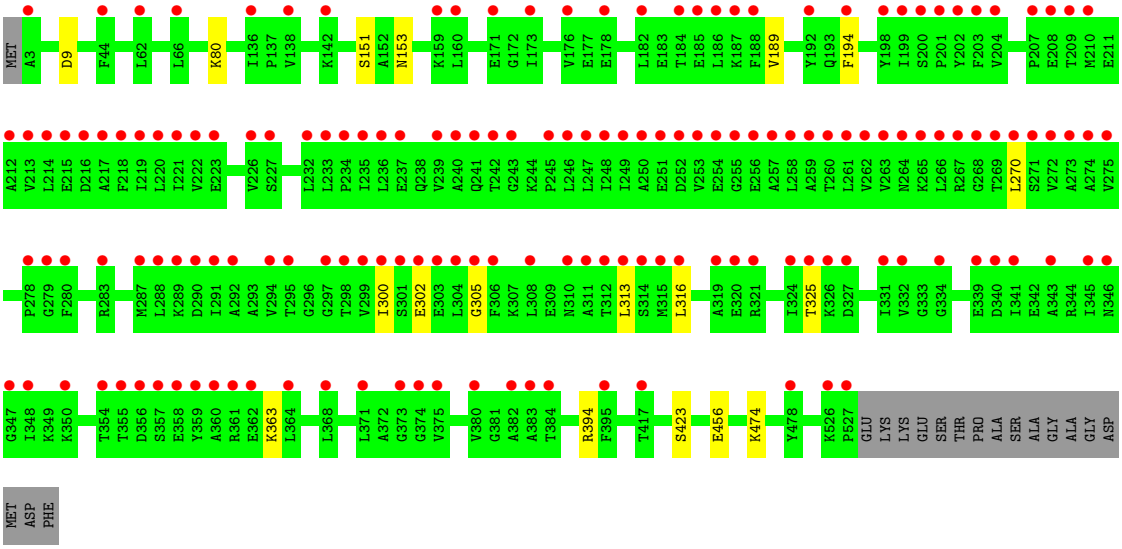




• Molecule 1: cpn60(GroEL)

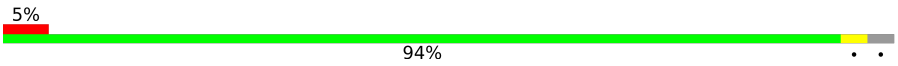
Chain m:

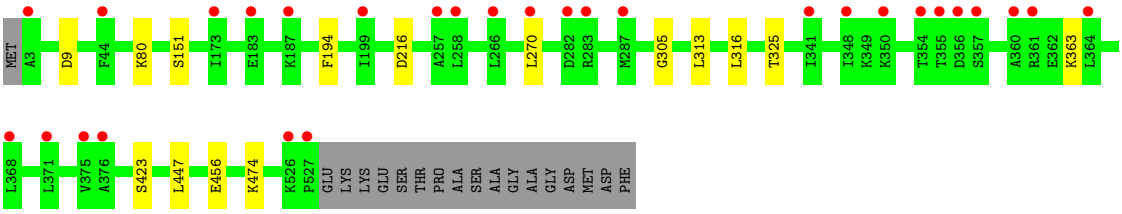




• Molecule 1: cpn60(GroEL)

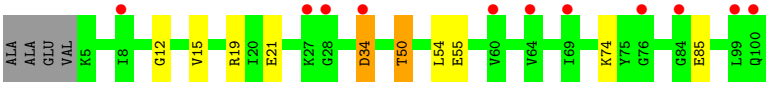
Chain n:



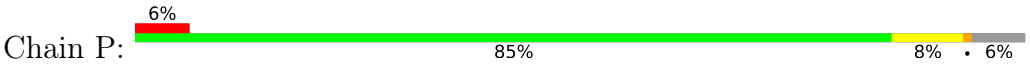


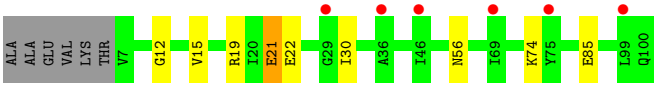
• Molecule 2: cpn10(GroES)

Chain O:

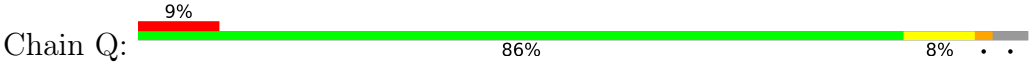


• Molecule 2: cpn10(GroES)

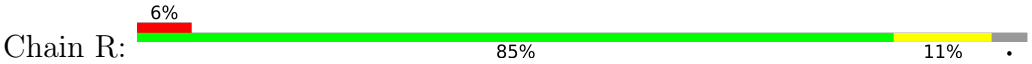


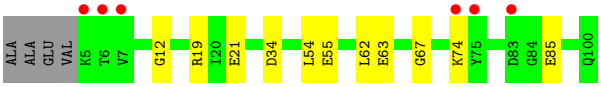


• Molecule 2: cpn10(GroES)

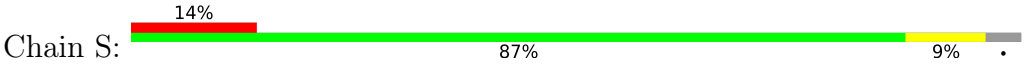


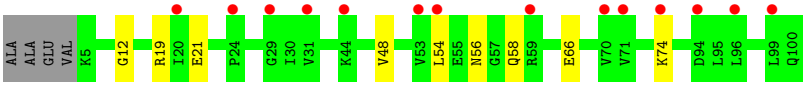
• Molecule 2: cpn10(GroES)



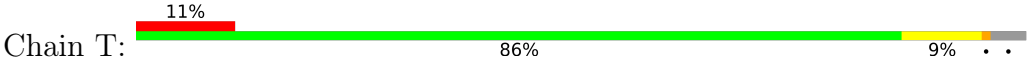


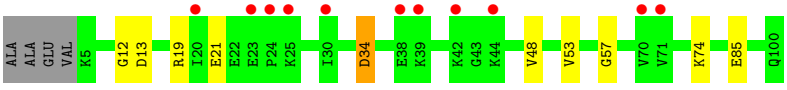
• Molecule 2: cpn10(GroES)



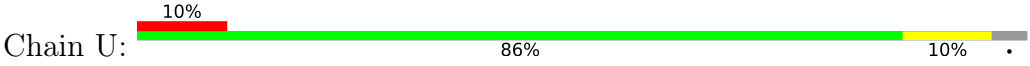


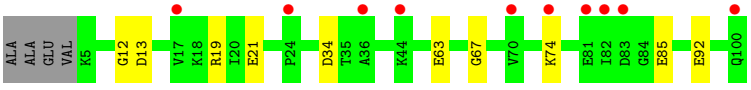
• Molecule 2: cpn10(GroES)





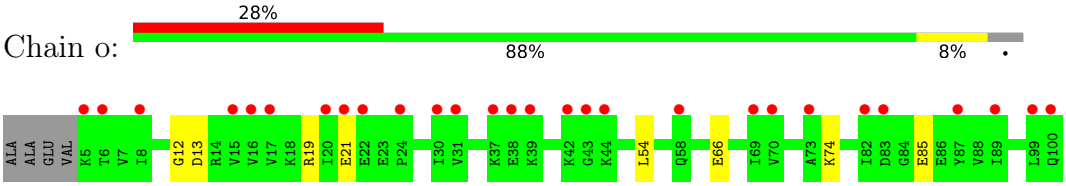
• Molecule 2: cpn10(GroES)





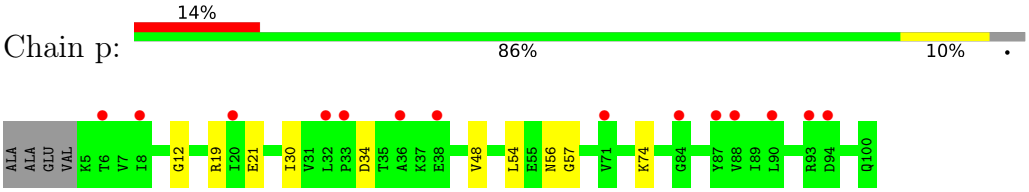
• Molecule 2: cpn10(GroES)

Chain o:



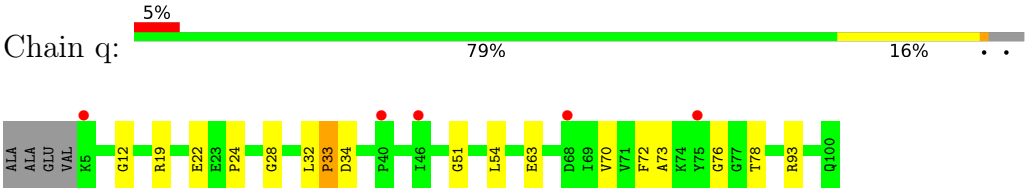
• Molecule 2: cpn10(GroES)

Chain p:



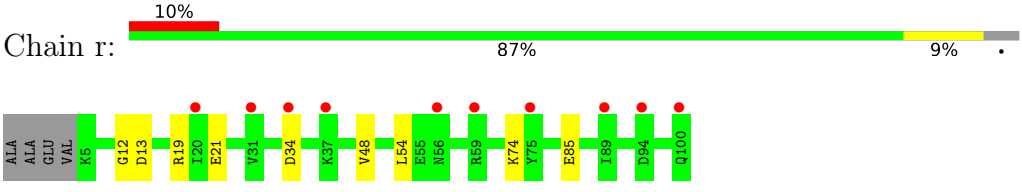
• Molecule 2: cpn10(GroES)

Chain q:



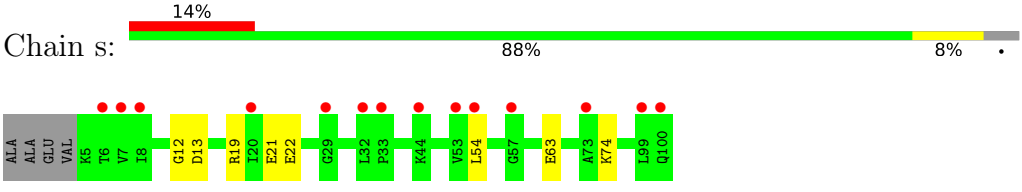
• Molecule 2: cpn10(GroES)

Chain r:



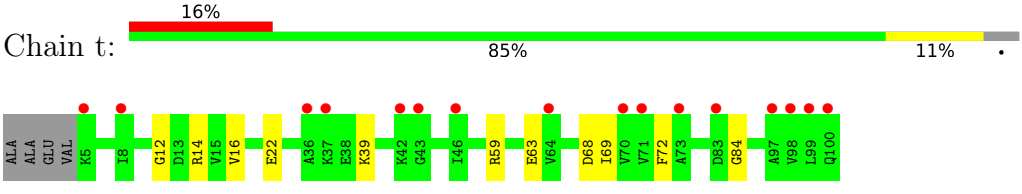
• Molecule 2: cpn10(GroES)

Chain s:



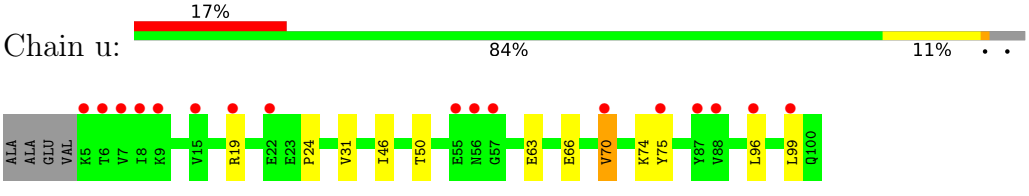
• Molecule 2: cpn10(GroES)

Chain t:



• Molecule 2: cpn10(GroES)

Chain u:



4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	1.35 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.239 , 0.279 0.233 , 0.272	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)	0.31 , 73.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.44	0/3989	0.65	0/5383
1	B	0.43	1/3989 (0.0%)	0.65	1/5383 (0.0%)
1	C	0.45	0/3980	0.67	0/5372
1	D	0.42	0/3980	0.65	1/5372 (0.0%)
1	E	0.43	0/3980	0.64	0/5372
1	F	0.39	0/4007	0.63	0/5406
1	G	0.41	0/3971	0.64	0/5360
1	H	0.36	0/3980	0.60	0/5372
1	I	0.37	0/3971	0.60	0/5360
1	J	0.40	0/3971	0.62	0/5360
1	K	0.39	1/3971 (0.0%)	0.62	0/5360
1	L	0.38	0/3980	0.60	0/5372
1	M	0.39	1/3971 (0.0%)	0.62	1/5360 (0.0%)
1	N	0.38	0/3980	0.63	1/5372 (0.0%)
1	a	0.41	0/3989	0.64	0/5383
1	b	0.40	0/3980	0.63	0/5372
1	c	0.39	0/3989	0.64	0/5383
1	d	0.39	0/3989	0.62	0/5383
1	e	0.37	0/3980	0.62	0/5372
1	f	0.34	0/3989	0.59	0/5383
1	g	0.41	1/3980 (0.0%)	0.62	1/5372 (0.0%)
1	h	0.40	0/3971	0.62	1/5360 (0.0%)
1	i	0.36	1/3971 (0.0%)	0.60	0/5360
1	j	0.35	0/3971	0.61	1/5360 (0.0%)
1	k	0.34	0/3971	0.59	0/5360
1	l	0.33	0/3971	0.59	0/5360
1	m	0.36	1/3971 (0.0%)	0.59	0/5360
1	n	0.34	0/3971	0.58	0/5360
2	O	0.40	0/746	0.68	0/1003
2	P	0.54	0/730	0.77	0/982
2	Q	0.39	0/746	0.70	2/1003 (0.2%)
2	R	0.42	0/746	0.69	0/1003

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
2	S	0.42	0/746	0.72	1/1003 (0.1%)
2	T	0.39	0/746	0.67	0/1003
2	U	0.46	0/746	0.72	0/1003
2	o	0.52	0/746	0.71	0/1003
2	p	0.40	0/746	0.68	0/1003
2	q	0.38	0/746	0.72	0/1003
2	r	0.41	0/746	0.67	0/1003
2	s	0.53	0/746	0.76	0/1003
2	t	0.31	0/746	0.64	0/1003
2	u	0.30	0/746	0.62	0/1003
All	All	0.39	6/121841 (0.0%)	0.63	10/164393 (0.0%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	133	ALA	CA-CB	-13.30	1.24	1.52
1	m	394	ARG	CZ-NH2	-8.93	1.21	1.33
1	K	237	GLU	CD-OE1	-5.26	1.19	1.25
1	M	512	ILE	CB-CG2	5.16	1.68	1.52
1	B	410	ILE	CB-CG2	5.08	1.68	1.52

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	444	ARG	NE-CZ-NH1	7.31	123.96	120.30
1	g	133	ALA	CB-CA-C	-7.31	99.13	110.10
1	j	283	ARG	CG-CD-NE	5.69	123.75	111.80
2	Q	51	GLY	N-CA-C	-5.32	99.81	113.10
1	M	512	ILE	CG1-CB-CG2	5.29	123.03	111.40

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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%)	5	19
1	B	525/543 (97%)	458 (87%)	55 (10%)	12 (2%)	6	21
1	C	524/543 (96%)	451 (86%)	58 (11%)	15 (3%)	4	15
1	D	524/543 (96%)	441 (84%)	67 (13%)	16 (3%)	4	14
1	E	524/543 (96%)	440 (84%)	65 (12%)	19 (4%)	3	11
1	F	527/543 (97%)	453 (86%)	60 (11%)	14 (3%)	5	17
1	G	523/543 (96%)	447 (86%)	65 (12%)	11 (2%)	7	23
1	H	524/543 (96%)	457 (87%)	60 (12%)	7 (1%)	12	36
1	I	523/543 (96%)	457 (87%)	61 (12%)	5 (1%)	15	44
1	J	523/543 (96%)	456 (87%)	58 (11%)	9 (2%)	9	29
1	K	523/543 (96%)	458 (88%)	57 (11%)	8 (2%)	10	33
1	L	524/543 (96%)	454 (87%)	63 (12%)	7 (1%)	12	36
1	M	523/543 (96%)	455 (87%)	61 (12%)	7 (1%)	12	36
1	N	524/543 (96%)	457 (87%)	61 (12%)	6 (1%)	14	41
1	a	525/543 (97%)	453 (86%)	57 (11%)	15 (3%)	4	15
1	b	524/543 (96%)	452 (86%)	61 (12%)	11 (2%)	7	23
1	c	525/543 (97%)	446 (85%)	61 (12%)	18 (3%)	3	13
1	d	525/543 (97%)	451 (86%)	56 (11%)	18 (3%)	3	13
1	e	524/543 (96%)	455 (87%)	57 (11%)	12 (2%)	6	21
1	f	525/543 (97%)	458 (87%)	55 (10%)	12 (2%)	6	21
1	g	524/543 (96%)	450 (86%)	60 (12%)	14 (3%)	5	17
1	h	523/543 (96%)	459 (88%)	57 (11%)	7 (1%)	12	36
1	i	523/543 (96%)	456 (87%)	58 (11%)	9 (2%)	9	29
1	j	523/543 (96%)	454 (87%)	60 (12%)	9 (2%)	9	29
1	k	523/543 (96%)	456 (87%)	61 (12%)	6 (1%)	14	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	l	523/543 (96%)	457 (87%)	59 (11%)	7 (1%)	12	36
1	m	523/543 (96%)	465 (89%)	51 (10%)	7 (1%)	12	36
1	n	523/543 (96%)	459 (88%)	58 (11%)	6 (1%)	14	41
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%)	1	1
2	S	94/100 (94%)	72 (77%)	17 (18%)	5 (5%)	2	6
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
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%)	2	6
2	t	94/100 (94%)	69 (73%)	17 (18%)	8 (8%)	1	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%)	5	19

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%)	49	81
1	B	412/423 (97%)	399 (97%)	13 (3%)	39	73
1	C	411/423 (97%)	399 (97%)	12 (3%)	42	76
1	D	411/423 (97%)	401 (98%)	10 (2%)	49	81
1	E	411/423 (97%)	395 (96%)	16 (4%)	32	66
1	F	414/423 (98%)	405 (98%)	9 (2%)	52	83
1	G	410/423 (97%)	400 (98%)	10 (2%)	49	81
1	H	411/423 (97%)	403 (98%)	8 (2%)	57	85
1	I	410/423 (97%)	400 (98%)	10 (2%)	49	81
1	J	410/423 (97%)	400 (98%)	10 (2%)	49	81
1	K	410/423 (97%)	401 (98%)	9 (2%)	52	83
1	L	411/423 (97%)	401 (98%)	10 (2%)	49	81
1	M	410/423 (97%)	399 (97%)	11 (3%)	44	78
1	N	411/423 (97%)	401 (98%)	10 (2%)	49	81
1	a	412/423 (97%)	404 (98%)	8 (2%)	57	85
1	b	411/423 (97%)	401 (98%)	10 (2%)	49	81
1	c	412/423 (97%)	400 (97%)	12 (3%)	42	76
1	d	412/423 (97%)	401 (97%)	11 (3%)	44	78
1	e	411/423 (97%)	403 (98%)	8 (2%)	57	85
1	f	412/423 (97%)	404 (98%)	8 (2%)	57	85
1	g	411/423 (97%)	401 (98%)	10 (2%)	49	81
1	h	410/423 (97%)	400 (98%)	10 (2%)	49	81
1	i	410/423 (97%)	399 (97%)	11 (3%)	44	78
1	j	410/423 (97%)	398 (97%)	12 (3%)	42	76
1	k	410/423 (97%)	399 (97%)	11 (3%)	44	78
1	l	410/423 (97%)	400 (98%)	10 (2%)	49	81
1	m	410/423 (97%)	400 (98%)	10 (2%)	49	81
1	n	410/423 (97%)	401 (98%)	9 (2%)	52	83
2	O	81/83 (98%)	76 (94%)	5 (6%)	18	47
2	P	79/83 (95%)	76 (96%)	3 (4%)	33	67
2	Q	81/83 (98%)	78 (96%)	3 (4%)	34	68
2	R	81/83 (98%)	78 (96%)	3 (4%)	34	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	S	81/83 (98%)	78 (96%)	3 (4%)	34	68
2	T	81/83 (98%)	77 (95%)	4 (5%)	25	57
2	U	81/83 (98%)	78 (96%)	3 (4%)	34	68
2	o	81/83 (98%)	79 (98%)	2 (2%)	47	80
2	p	81/83 (98%)	78 (96%)	3 (4%)	34	68
2	q	81/83 (98%)	78 (96%)	3 (4%)	34	68
2	r	81/83 (98%)	78 (96%)	3 (4%)	34	68
2	s	81/83 (98%)	78 (96%)	3 (4%)	34	68
2	t	81/83 (98%)	78 (96%)	3 (4%)	34	68
2	u	81/83 (98%)	78 (96%)	3 (4%)	34	68
All	All	12637/13006 (97%)	12305 (97%)	332 (3%)	46	79

5 of 332 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	g	36	ARG
1	l	194	PHE
1	g	342	GLU
1	j	151	SER
1	m	363	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 271 such sidechains are listed below:

Mol	Chain	Res	Type
1	l	310	ASN
1	l	508	ASN
1	n	400	ASN
1	L	228	ASN
1	L	97	GLN

5.3.3 RNA

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 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	J	601	-	3,3,3	0.37	0	3,3,3	0.75	0
5	DMS	N	701	-	3,3,3	0.25	0	3,3,3	0.66	0
4	ADP	e	602	3	24,29,29	1.68	5 (20%)	29,45,45	1.64	3 (10%)
4	ADP	g	602	3	24,29,29	1.51	5 (20%)	29,45,45	1.57	3 (10%)
5	DMS	I	601	-	3,3,3	0.26	0	3,3,3	0.68	0
5	DMS	j	601	-	3,3,3	0.29	0	3,3,3	0.66	0
4	ADP	B	602	3	24,29,29	1.48	4 (16%)	29,45,45	1.56	3 (10%)
4	ADP	D	602	3	24,29,29	1.65	6 (25%)	29,45,45	1.56	2 (6%)
5	DMS	i	601	-	3,3,3	0.33	0	3,3,3	0.71	0
4	ADP	a	602	3	24,29,29	1.60	4 (16%)	29,45,45	1.57	3 (10%)
5	DMS	L	601	-	3,3,3	0.31	0	3,3,3	0.69	0
5	DMS	k	601	-	3,3,3	0.30	0	3,3,3	0.67	0
5	DMS	K	601	-	3,3,3	0.29	0	3,3,3	0.69	0
5	DMS	l	601	-	3,3,3	0.33	0	3,3,3	0.68	0
4	ADP	G	602	3	24,29,29	1.49	6 (25%)	29,45,45	1.61	3 (10%)
5	DMS	m	601	-	3,3,3	0.26	0	3,3,3	0.62	0
4	ADP	E	602	3	24,29,29	1.40	5 (20%)	29,45,45	1.65	4 (13%)
4	ADP	c	602	3	24,29,29	1.61	4 (16%)	29,45,45	1.74	3 (10%)
4	ADP	b	602	3	24,29,29	1.71	5 (20%)	29,45,45	1.63	2 (6%)
5	DMS	h	601	-	3,3,3	0.35	0	3,3,3	0.71	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	ADP	d	602	3	24,29,29	1.65	6 (25%)	29,45,45	1.63	4 (13%)
4	ADP	F	602	3	24,29,29	1.53	4 (16%)	29,45,45	1.58	3 (10%)
5	DMS	M	601	-	3,3,3	0.28	0	3,3,3	0.64	0
4	ADP	f	602	3	24,29,29	1.56	5 (20%)	29,45,45	1.60	3 (10%)
5	DMS	H	601	-	3,3,3	0.22	0	3,3,3	0.67	0
5	DMS	n	701	-	3,3,3	0.25	0	3,3,3	0.62	0
4	ADP	A	602	3	24,29,29	1.41	4 (16%)	29,45,45	1.57	3 (10%)
4	ADP	C	602	3	24,29,29	1.54	3 (12%)	29,45,45	1.61	3 (10%)

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	E	602	3	-	8/12/32/32	0/3/3/3
4	ADP	c	602	3	-	8/12/32/32	0/3/3/3
4	ADP	F	602	3	-	7/12/32/32	0/3/3/3
4	ADP	B	602	3	-	7/12/32/32	0/3/3/3
4	ADP	D	602	3	-	8/12/32/32	0/3/3/3
4	ADP	b	602	3	-	8/12/32/32	0/3/3/3
4	ADP	e	602	3	-	7/12/32/32	0/3/3/3
4	ADP	a	602	3	-	7/12/32/32	0/3/3/3
4	ADP	f	602	3	-	8/12/32/32	0/3/3/3
4	ADP	g	602	3	-	8/12/32/32	0/3/3/3
4	ADP	A	602	3	-	6/12/32/32	0/3/3/3
4	ADP	d	602	3	-	6/12/32/32	0/3/3/3
4	ADP	C	602	3	-	7/12/32/32	0/3/3/3
4	ADP	G	602	3	-	7/12/32/32	0/3/3/3

The worst 5 of 66 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	602	ADP	C2'-C1'	-4.59	1.46	1.53
4	C	602	ADP	C2'-C1'	-4.32	1.47	1.53
4	F	602	ADP	C2'-C1'	-4.26	1.47	1.53
4	a	602	ADP	C2'-C1'	-4.22	1.47	1.53
4	D	602	ADP	C2-N3	4.20	1.38	1.32

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	c	602	ADP	N3-C2-N1	-7.15	117.50	128.68
4	f	602	ADP	N3-C2-N1	-7.01	117.72	128.68
4	b	602	ADP	N3-C2-N1	-6.98	117.77	128.68
4	d	602	ADP	N3-C2-N1	-6.97	117.78	128.68
4	C	602	ADP	N3-C2-N1	-6.92	117.86	128.68

There are no chirality outliers.

5 of 102 torsion outliers are listed below:

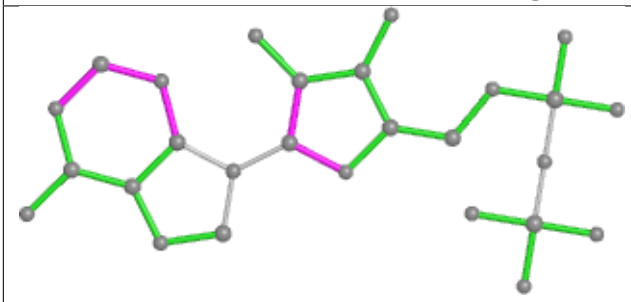
Mol	Chain	Res	Type	Atoms
4	A	602	ADP	C5'-O5'-PA-O1A
4	A	602	ADP	C5'-O5'-PA-O2A
4	A	602	ADP	C5'-O5'-PA-O3A
4	A	602	ADP	O4'-C4'-C5'-O5'
4	B	602	ADP	C5'-O5'-PA-O1A

There are no ring outliers.

No monomer is involved in short contacts.

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 e 602



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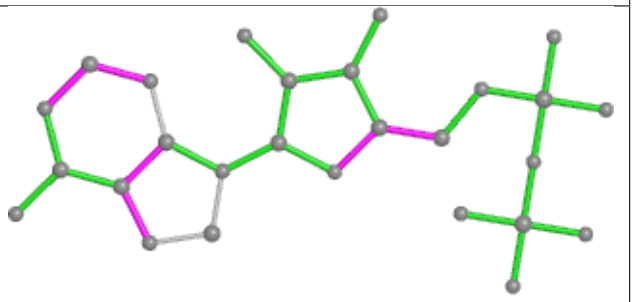

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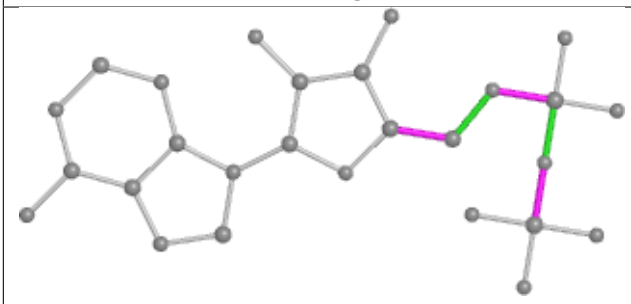

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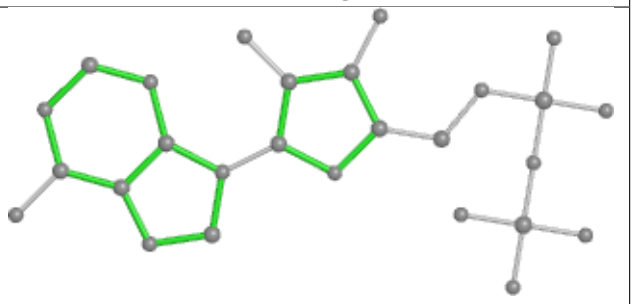
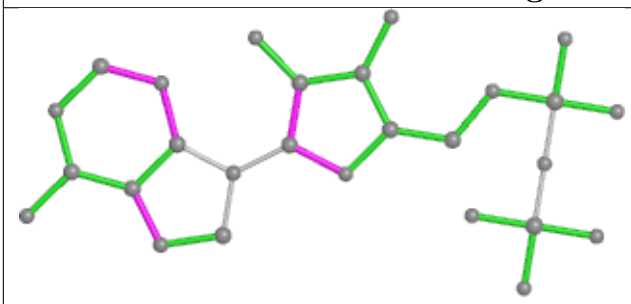


Rings

Ligand ADP g 602



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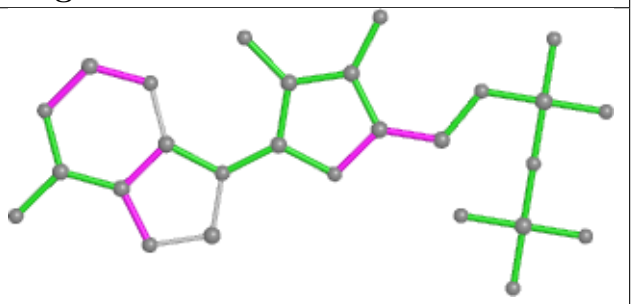

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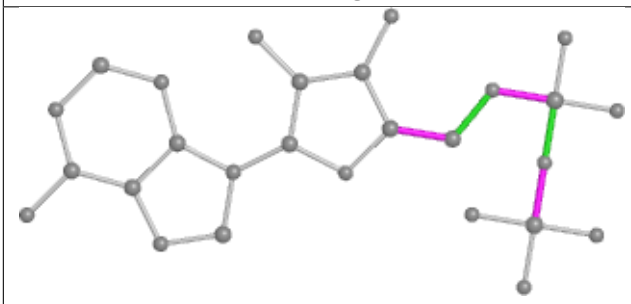

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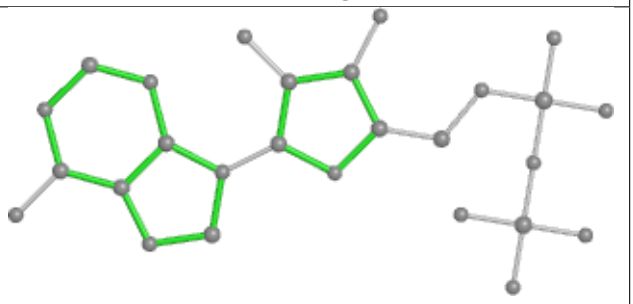
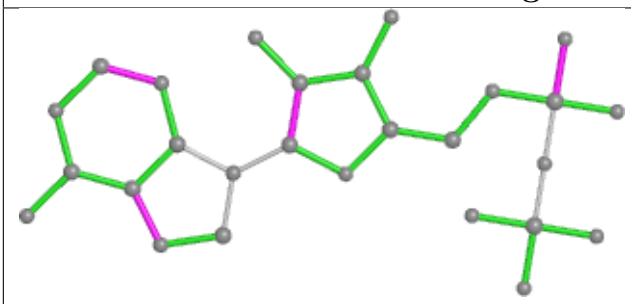


Rings

Ligand ADP B 602



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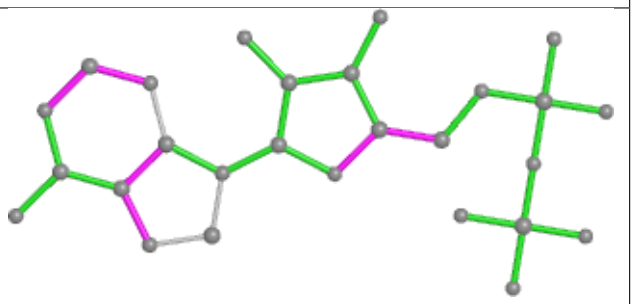

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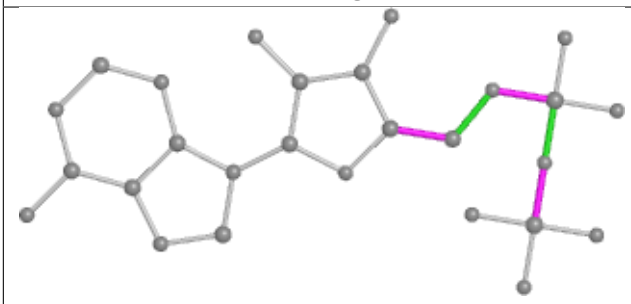

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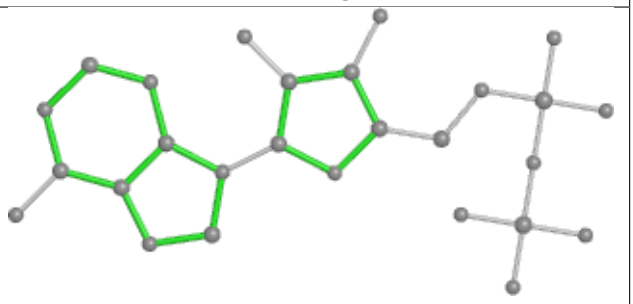

Rings

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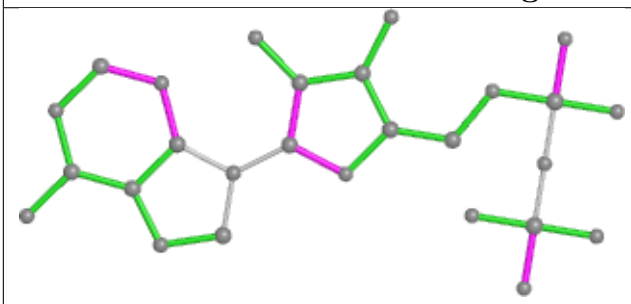

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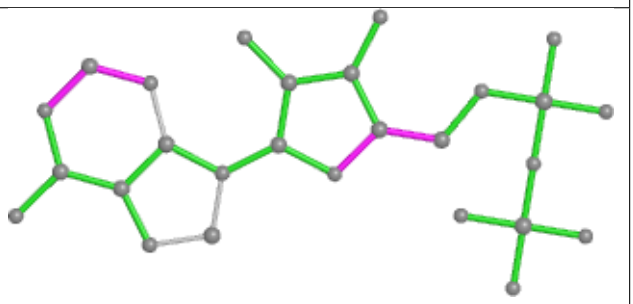

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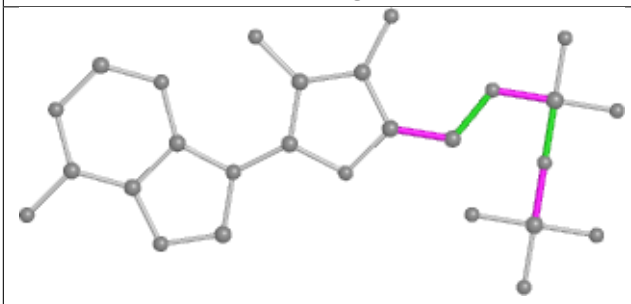

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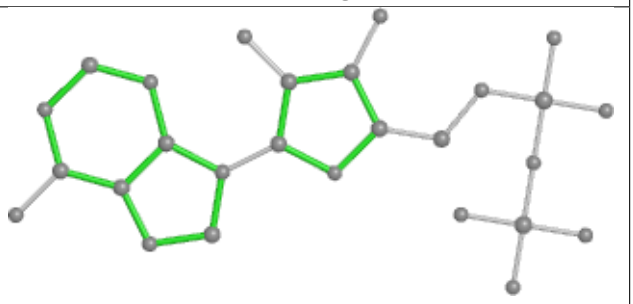
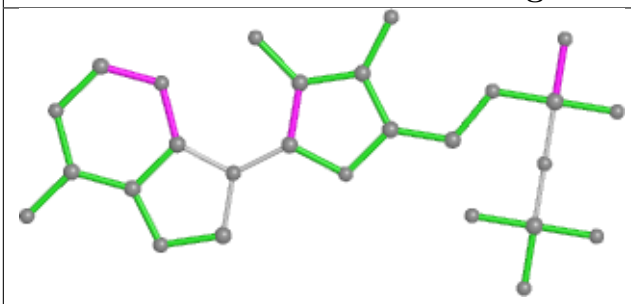


Rings

Ligand ADP a 602



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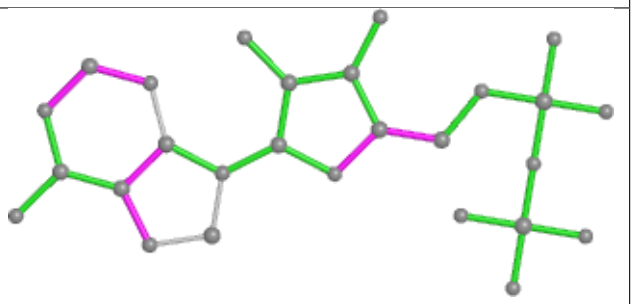

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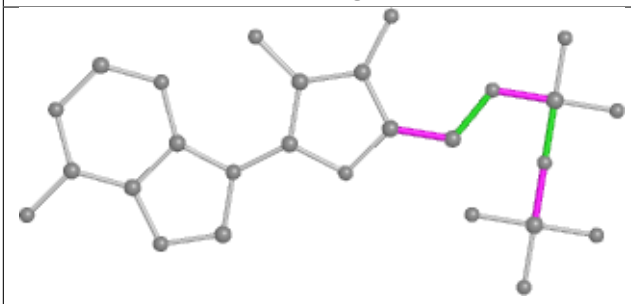

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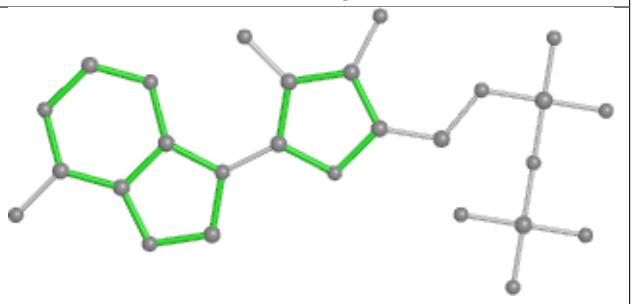

Rings

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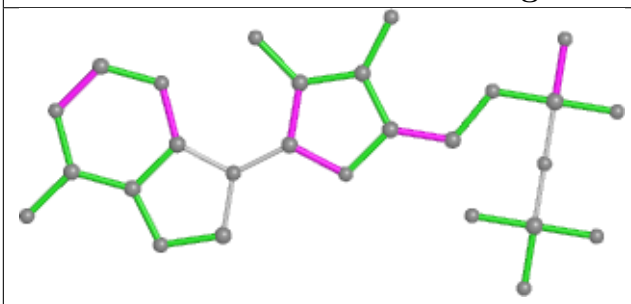

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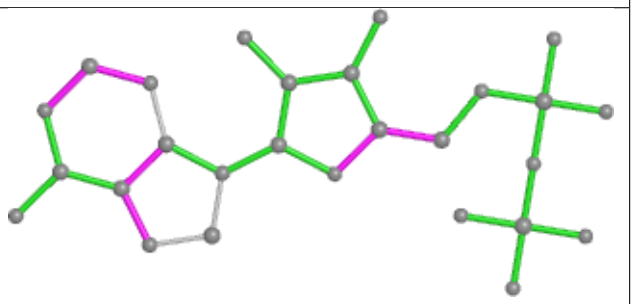

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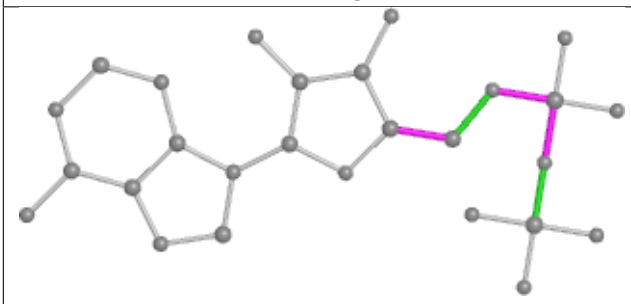

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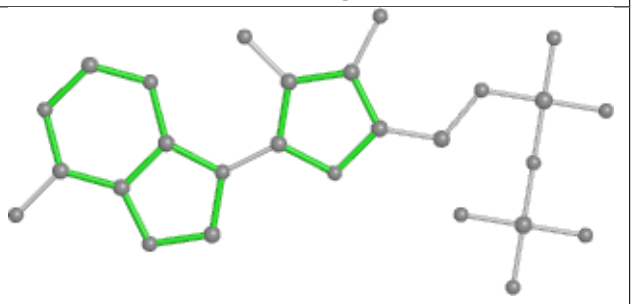

Rings

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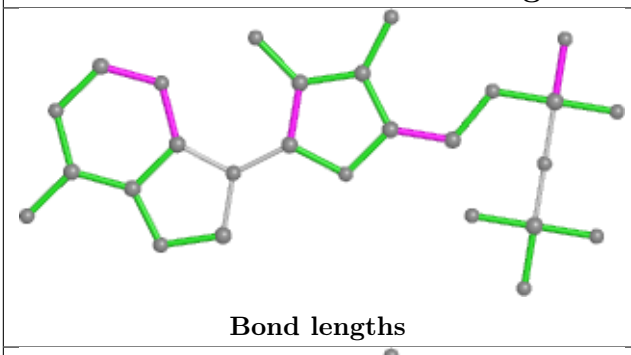

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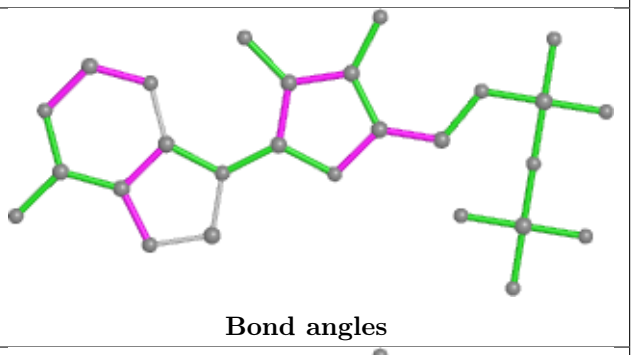

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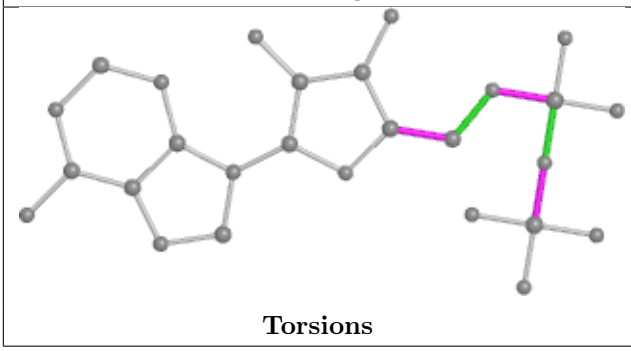

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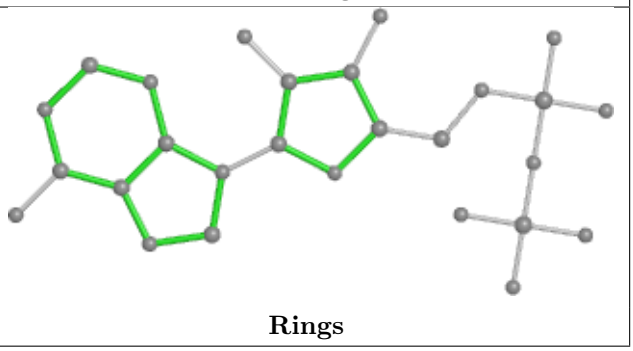
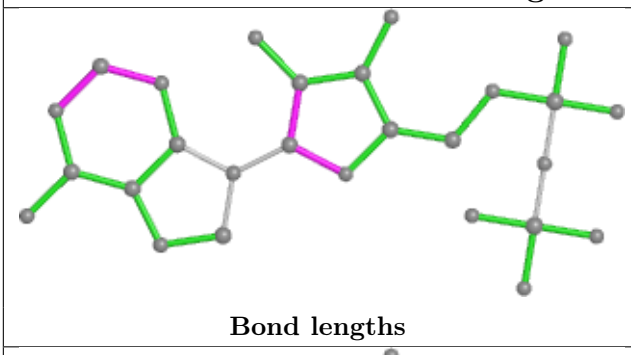


Rings

Ligand ADP c 602



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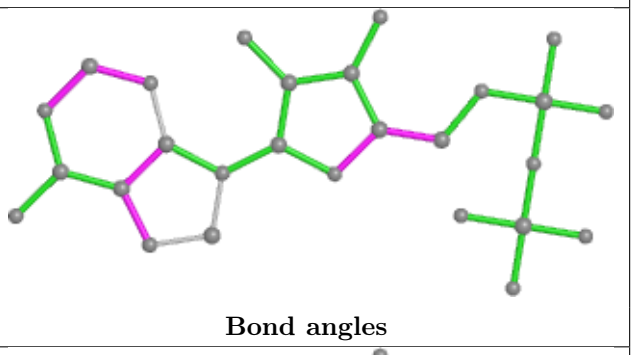

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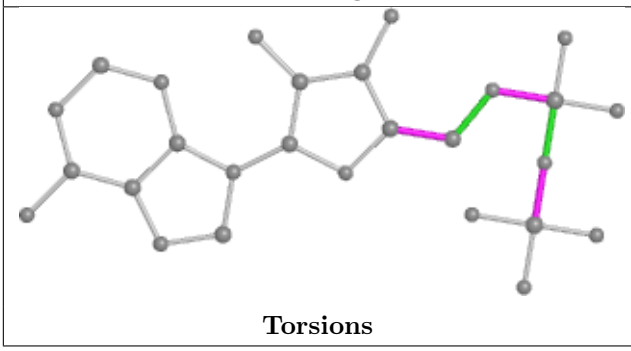

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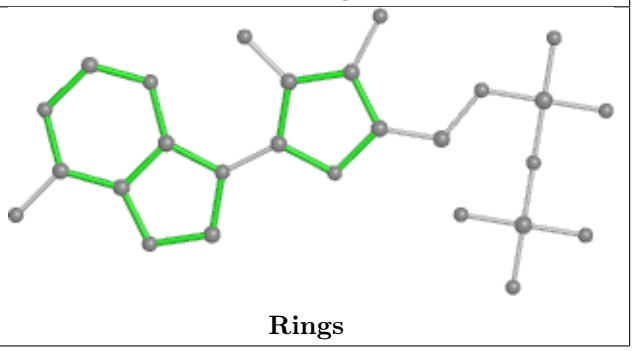
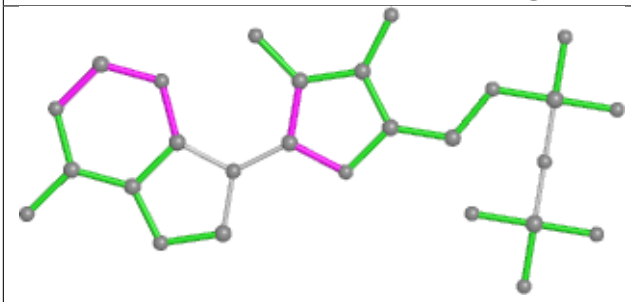
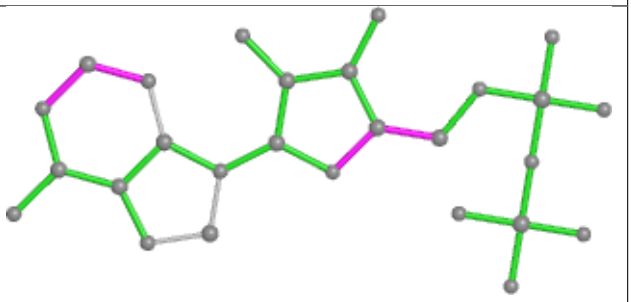
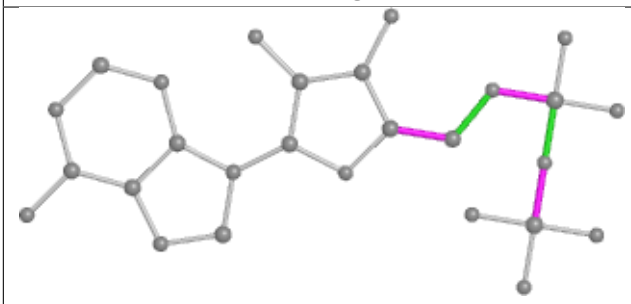
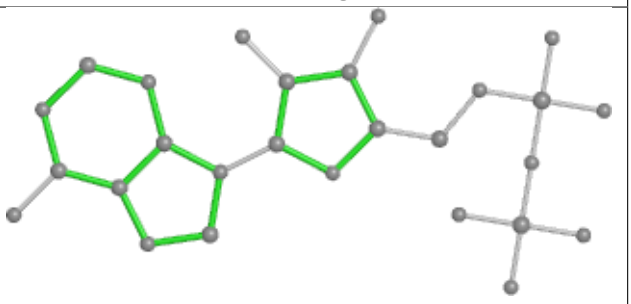
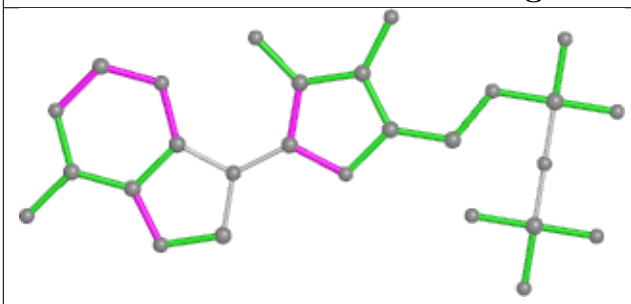
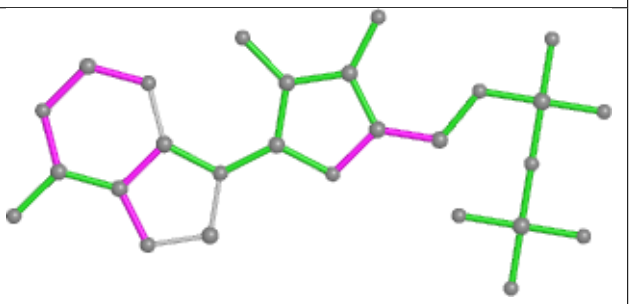
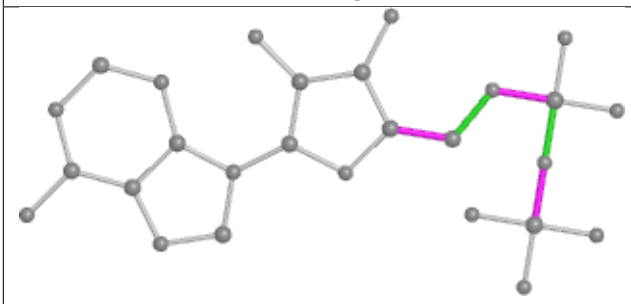
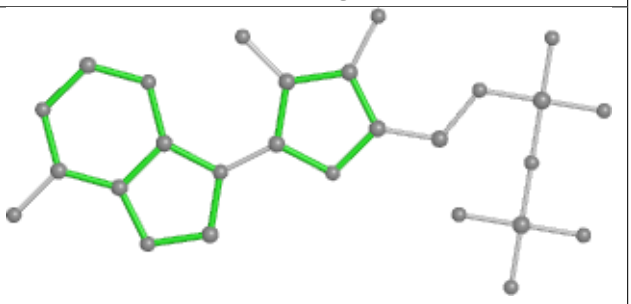
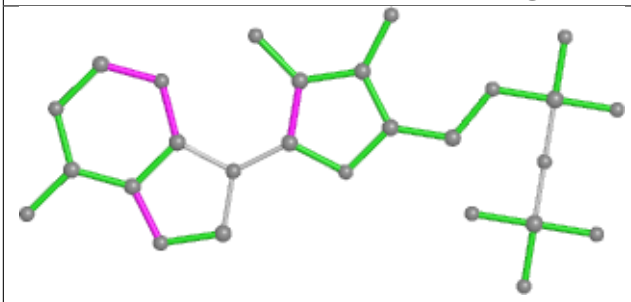


Rings

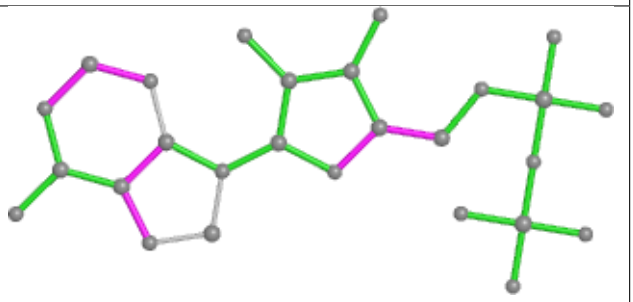
Ligand ADP b 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP d 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

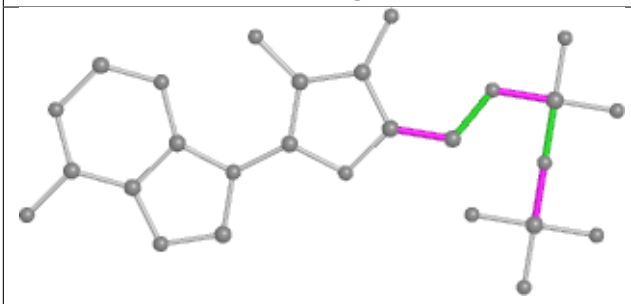
Ligand ADP F 602



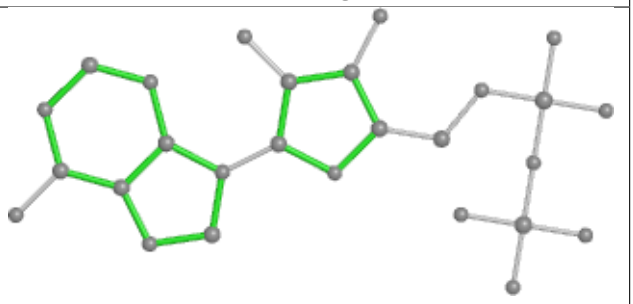
Bond lengths



Bond angles

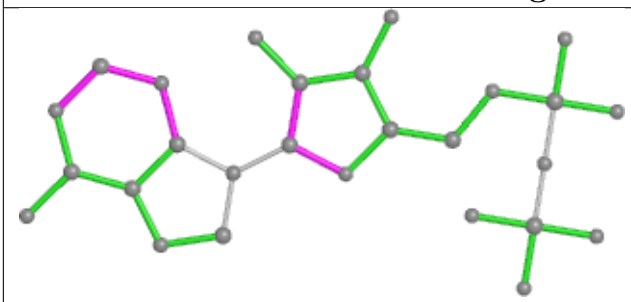


Torsions

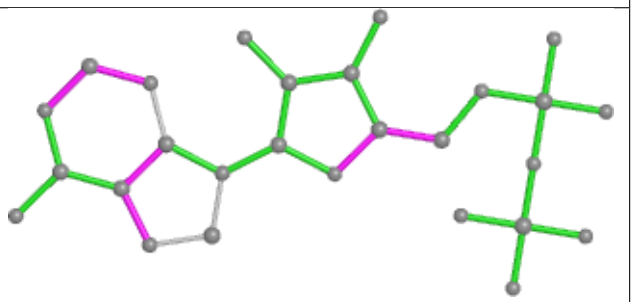


Rings

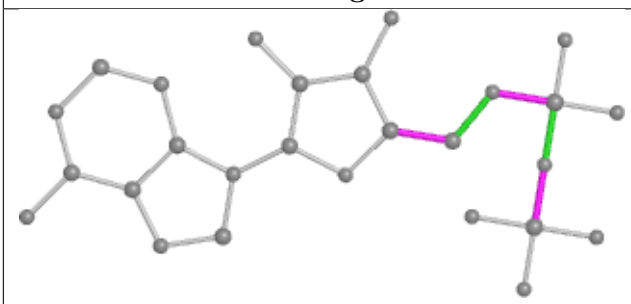
Ligand ADP f 602



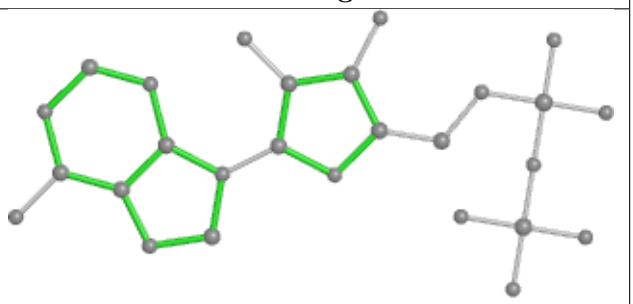
Bond lengths



Bond angles

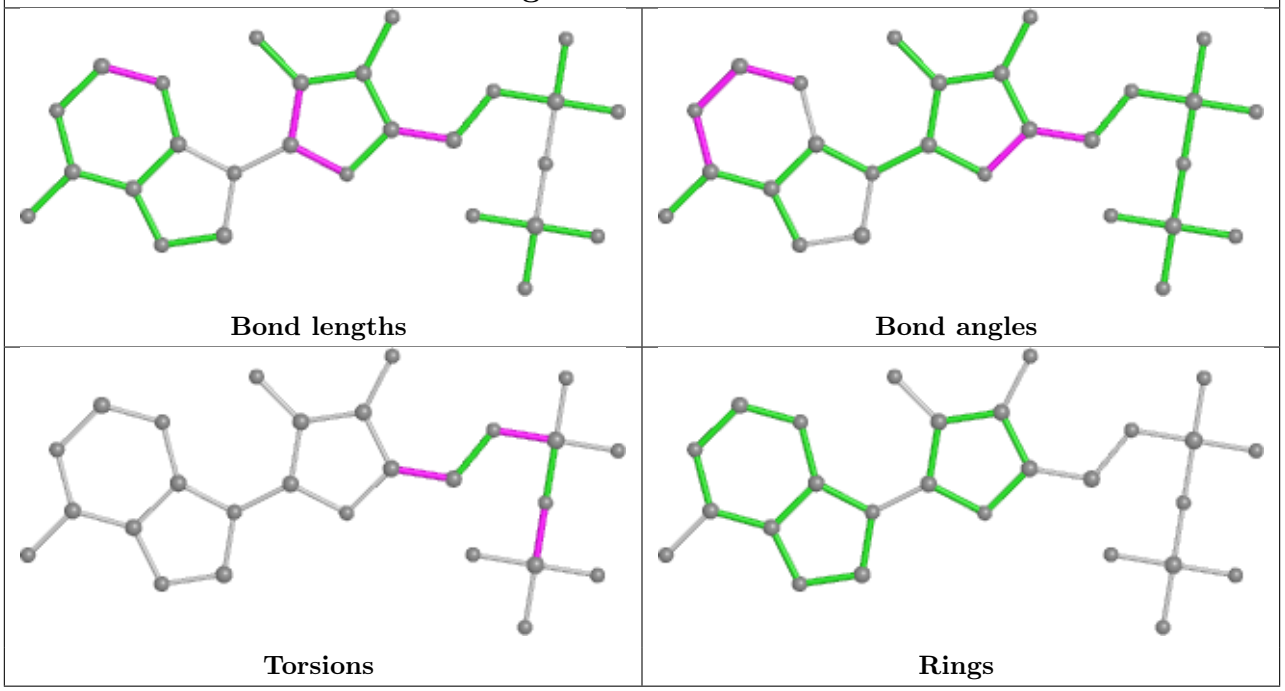


Torsions

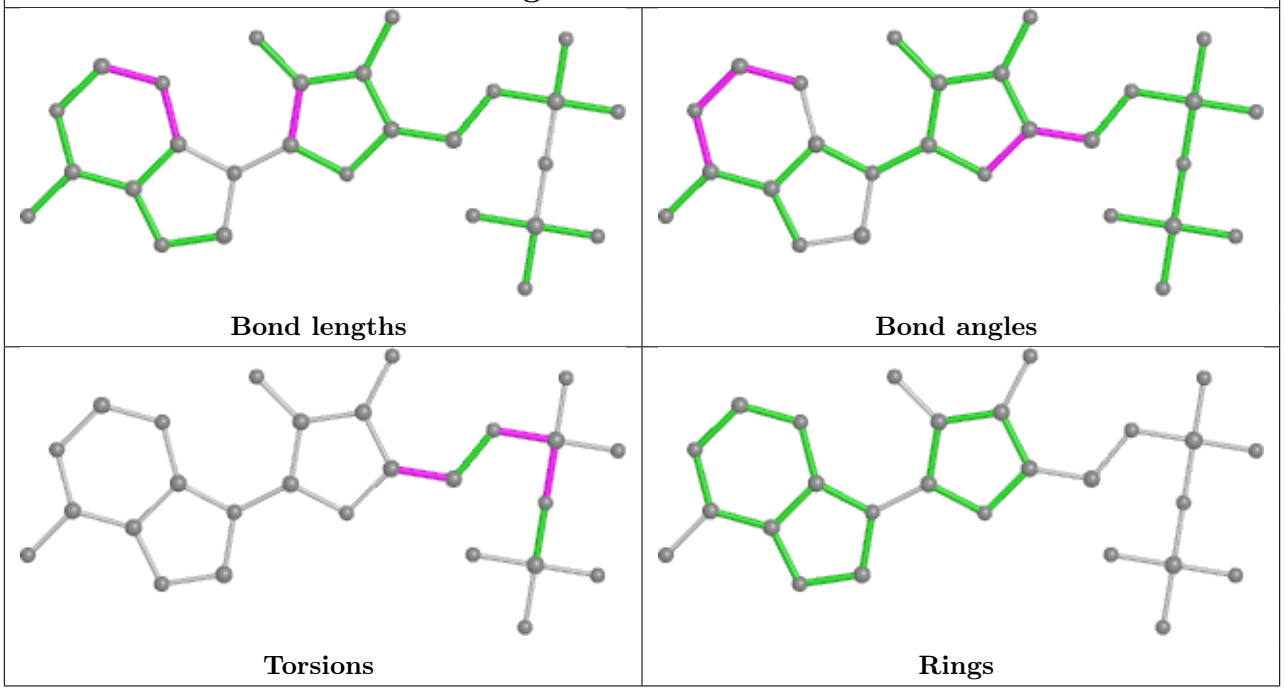


Rings

Ligand ADP A 602



Ligand ADP C 602



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	-0.22	4 (0%)	86	81	16, 51, 95, 147	0
1	B	527/543 (97%)	-0.17	5 (0%)	84	80	15, 52, 101, 146	0
1	C	526/543 (96%)	-0.24	2 (0%)	92	91	14, 50, 101, 140	0
1	D	526/543 (96%)	-0.09	11 (2%)	63	54	14, 55, 120, 154	0
1	E	526/543 (96%)	-0.03	12 (2%)	60	51	9, 51, 127, 164	0
1	F	529/543 (97%)	-0.08	9 (1%)	70	63	17, 58, 108, 159	0
1	G	525/543 (96%)	-0.14	4 (0%)	86	81	19, 57, 106, 140	0
1	H	526/543 (96%)	-0.03	14 (2%)	54	44	26, 70, 120, 163	0
1	I	525/543 (96%)	-0.10	9 (1%)	70	63	24, 67, 121, 151	0
1	J	525/543 (96%)	-0.13	8 (1%)	73	68	14, 55, 110, 163	0
1	K	525/543 (96%)	-0.08	11 (2%)	63	54	16, 63, 120, 157	0
1	L	526/543 (96%)	-0.09	10 (1%)	66	59	23, 62, 115, 154	0
1	M	525/543 (96%)	1.90	181 (34%)	0	0	25, 95, 150, 167	0
1	N	526/543 (96%)	0.07	22 (4%)	36	26	25, 70, 124, 167	0
1	a	527/543 (97%)	0.26	37 (7%)	16	9	18, 71, 128, 157	0
1	b	526/543 (96%)	0.21	47 (8%)	9	5	18, 66, 121, 163	0
1	c	527/543 (97%)	0.14	28 (5%)	26	17	23, 72, 134, 166	0
1	d	527/543 (97%)	0.03	12 (2%)	60	51	29, 77, 118, 146	0
1	e	526/543 (96%)	0.16	20 (3%)	40	30	42, 81, 116, 155	0
1	f	527/543 (97%)	0.30	25 (4%)	31	22	45, 88, 123, 149	0
1	g	526/543 (96%)	0.21	31 (5%)	22	14	27, 88, 136, 163	0
1	h	525/543 (96%)	-0.08	7 (1%)	77	72	24, 61, 112, 150	0
1	i	525/543 (96%)	0.09	25 (4%)	30	21	28, 76, 125, 160	0
1	j	525/543 (96%)	0.22	29 (5%)	25	16	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%)	0.49	60 (11%) 5 3	37, 94, 135, 158	0
1	l	525/543 (96%)	1.00	110 (20%) 1 0	48, 106, 143, 162	0
1	m	525/543 (96%)	1.52	161 (30%) 0 0	56, 104, 146, 174	0
1	n	525/543 (96%)	0.10	29 (5%) 25 16	37, 79, 130, 158	0
2	O	96/100 (96%)	0.62	11 (11%) 4 2	59, 109, 142, 146	0
2	P	94/100 (94%)	0.52	6 (6%) 19 12	69, 108, 142, 146	0
2	Q	96/100 (96%)	0.61	9 (9%) 8 4	60, 108, 142, 149	0
2	R	96/100 (96%)	0.41	6 (6%) 20 12	60, 99, 134, 151	0
2	S	96/100 (96%)	0.75	14 (14%) 2 1	61, 107, 140, 150	0
2	T	96/100 (96%)	0.74	11 (11%) 4 2	65, 106, 141, 154	0
2	U	96/100 (96%)	0.71	10 (10%) 6 3	55, 107, 142, 148	0
2	o	96/100 (96%)	1.39	28 (29%) 0 0	86, 116, 152, 164	0
2	p	96/100 (96%)	0.82	14 (14%) 2 1	80, 112, 146, 150	0
2	q	96/100 (96%)	0.49	5 (5%) 27 18	45, 101, 141, 157	0
2	r	96/100 (96%)	0.66	10 (10%) 6 3	60, 109, 141, 150	0
2	s	96/100 (96%)	0.82	14 (14%) 2 1	73, 114, 143, 150	0
2	t	96/100 (96%)	0.68	16 (16%) 1 1	82, 118, 147, 159	0
2	u	96/100 (96%)	0.89	17 (17%) 1 1	83, 122, 153, 167	0
All	All	16067/16604 (96%)	0.23	1094 (6%) 17 10	9, 76, 133, 174	0

The worst 5 of 1094 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	294	VAL	17.1
1	M	291	ILE	16.7
1	M	273	ALA	16.4
1	M	247	LEU	15.1
1	M	246	LEU	13.3

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
3	MG	d	601	1/1	0.72	0.39	68,68,68,68	0
5	DMS	j	601	4/4	0.78	0.28	82,83,101,117	0
3	MG	e	601	1/1	0.83	0.31	62,62,62,62	0
5	DMS	J	601	4/4	0.84	0.24	39,53,65,90	0
5	DMS	n	701	4/4	0.87	0.27	69,85,87,99	0
5	DMS	k	601	4/4	0.88	0.25	89,96,103,115	0
5	DMS	l	601	4/4	0.88	0.24	63,95,106,125	0
3	MG	c	601	1/1	0.88	0.33	51,51,51,51	0
3	MG	b	601	1/1	0.89	0.27	53,53,53,53	0
5	DMS	K	601	4/4	0.90	0.18	43,44,76,91	0
5	DMS	L	601	4/4	0.90	0.24	39,58,61,94	0
5	DMS	H	601	4/4	0.91	0.24	24,28,74,96	0
4	ADP	f	602	27/27	0.91	0.28	47,93,109,116	0
4	ADP	g	602	27/27	0.92	0.26	56,84,98,103	0
3	MG	f	601	1/1	0.92	0.49	70,70,70,70	0
3	MG	C	601	1/1	0.92	0.21	28,28,28,28	0
5	DMS	h	601	4/4	0.93	0.22	52,58,85,96	0
3	MG	A	601	1/1	0.93	0.25	27,27,27,27	0
3	MG	g	601	1/1	0.93	0.53	66,66,66,66	0
4	ADP	d	602	27/27	0.93	0.23	45,72,87,93	0
5	DMS	m	601	4/4	0.93	0.23	82,92,95,105	0
5	DMS	M	601	4/4	0.93	0.20	26,29,60,79	0
4	ADP	a	602	27/27	0.94	0.24	21,70,81,90	0
4	ADP	c	602	27/27	0.94	0.23	24,67,80,102	0
3	MG	D	601	1/1	0.94	0.23	29,29,29,29	0
4	ADP	e	602	27/27	0.94	0.23	48,78,103,108	0
5	DMS	i	601	4/4	0.94	0.22	27,32,40,87	0
3	MG	B	601	1/1	0.95	0.32	44,44,44,44	0
3	MG	E	601	1/1	0.95	0.22	20,20,20,20	0
3	MG	a	601	1/1	0.95	0.34	54,54,54,54	0
5	DMS	I	601	4/4	0.95	0.20	37,58,66,93	0
4	ADP	D	602	27/27	0.95	0.20	1,38,64,69	0

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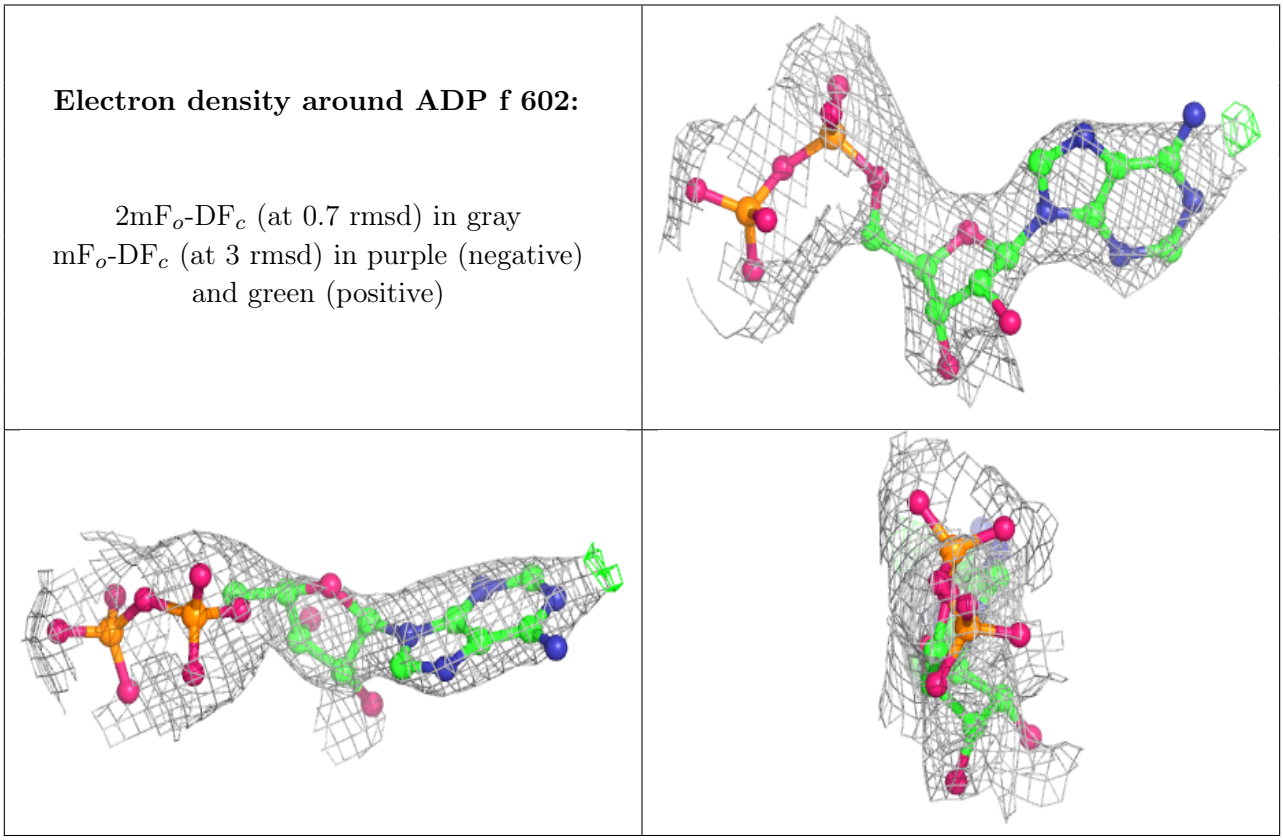
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	ADP	C	602	27/27	0.96	0.19	1,34,70,78	0
3	MG	F	601	1/1	0.96	0.27	25,25,25,25	0
4	ADP	E	602	27/27	0.96	0.20	12,44,74,80	0
4	ADP	G	602	27/27	0.96	0.21	1,61,76,85	0
4	ADP	B	602	27/27	0.96	0.23	18,54,75,80	0
4	ADP	b	602	27/27	0.96	0.20	13,58,79,85	0
3	MG	G	601	1/1	0.97	0.21	29,29,29,29	0
4	ADP	A	602	27/27	0.97	0.21	1,47,68,77	0
4	ADP	F	602	27/27	0.97	0.21	23,51,75,88	0
5	DMS	N	701	4/4	0.98	0.16	53,57,64,90	0

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

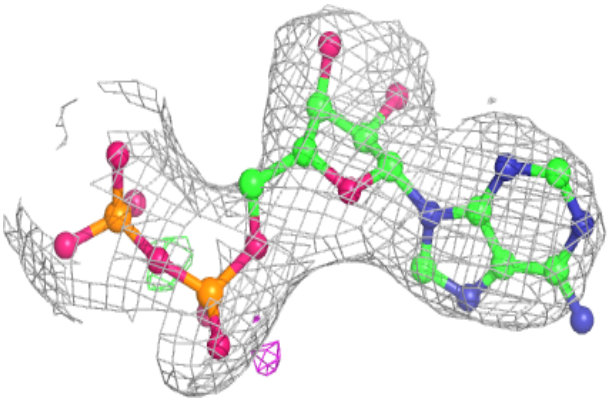
Electron density around ADP f 602:

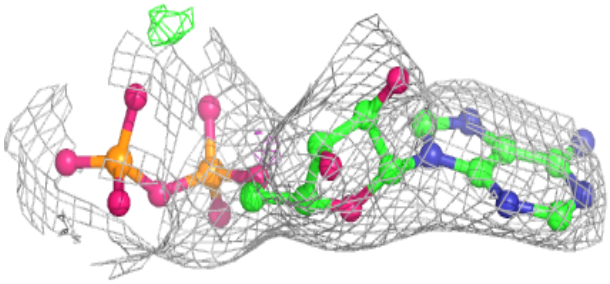
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

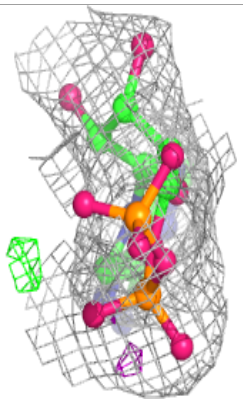


Electron density around ADP g 602:

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

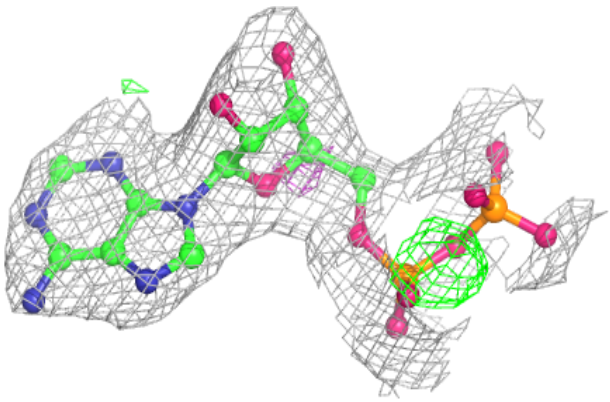


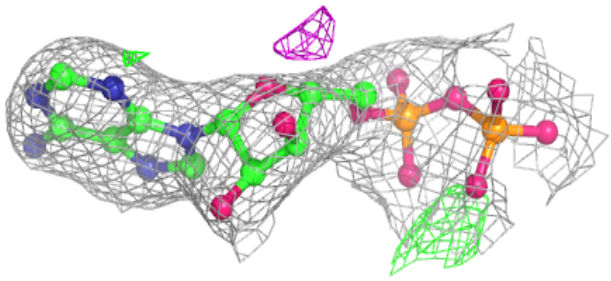


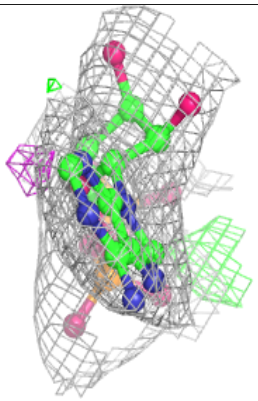


Electron density around ADP d 602:

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

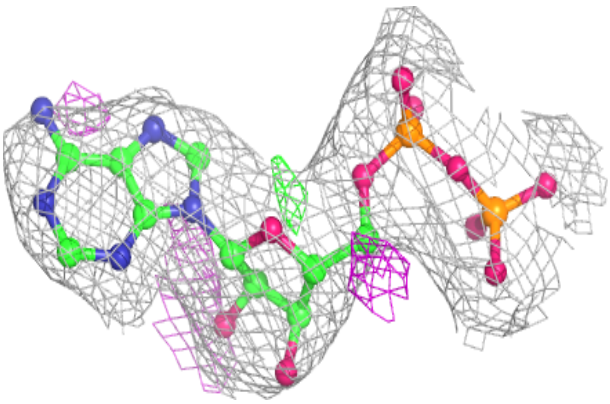


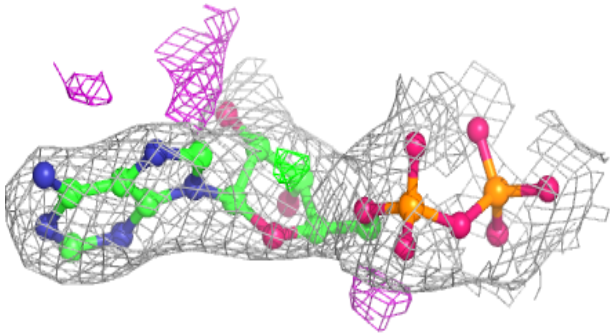


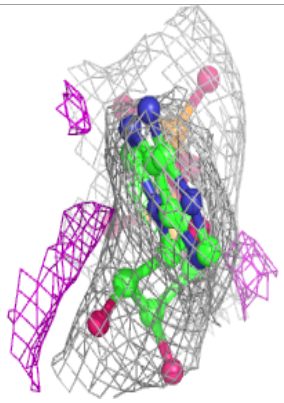


Electron density around ADP a 602:

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

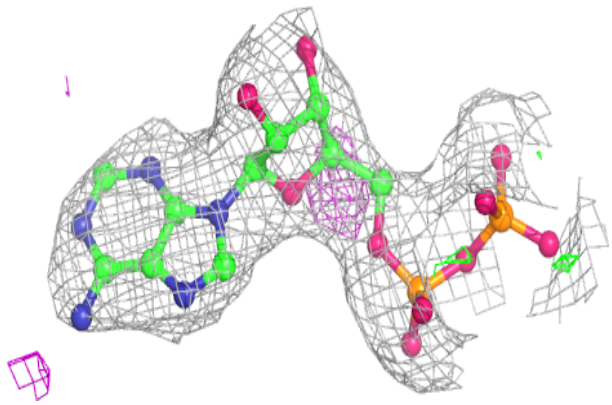


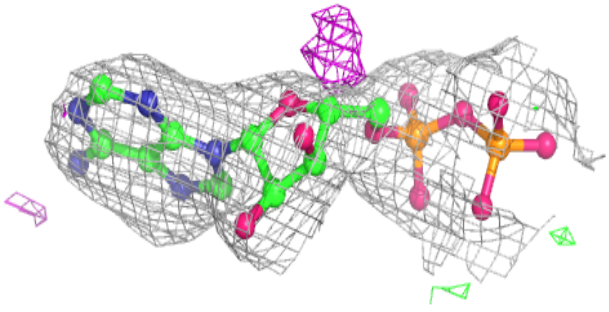


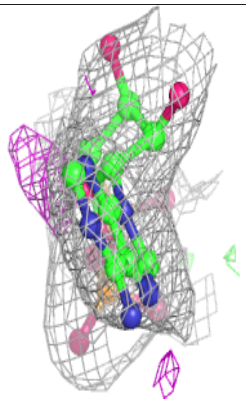


Electron density around ADP c 602:

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

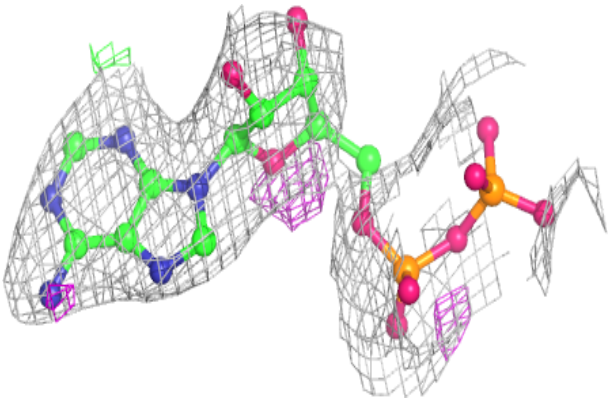


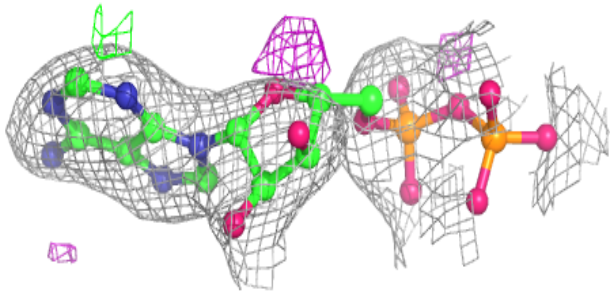


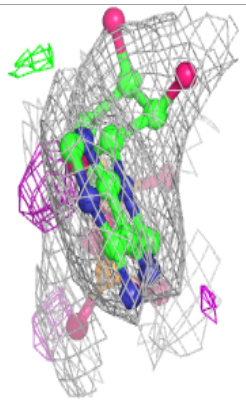


Electron density around ADP e 602:

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

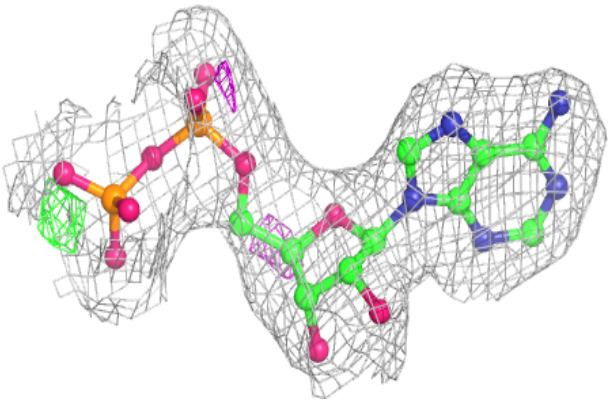


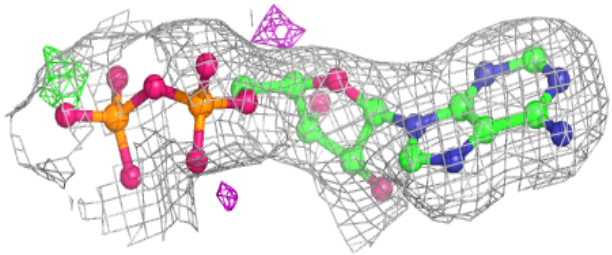


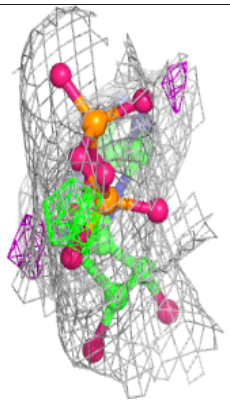


Electron density around ADP D 602:

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

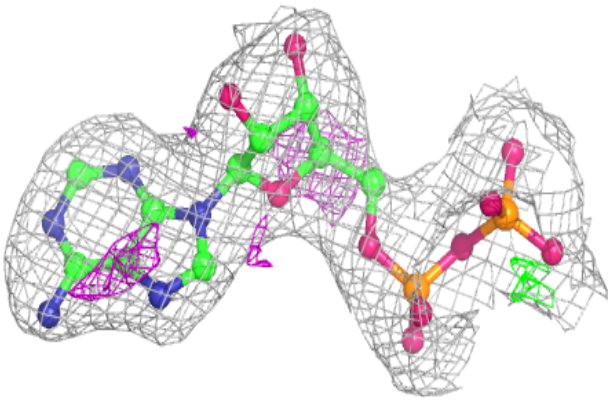


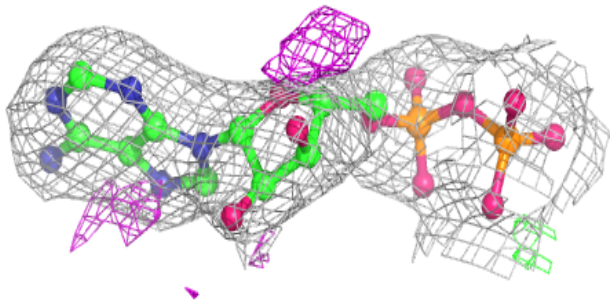


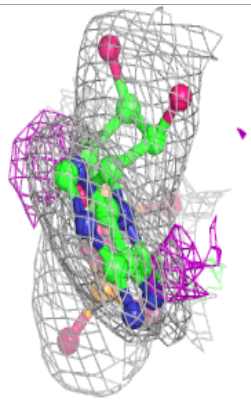


Electron density around ADP C 602:

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

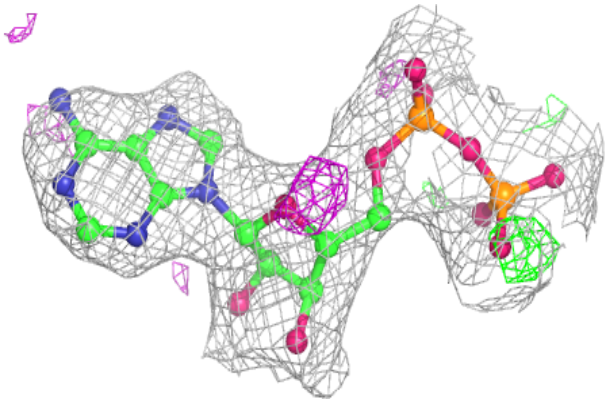


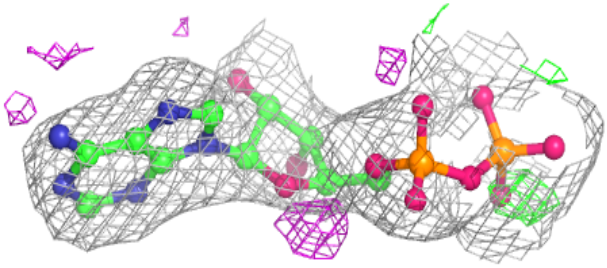


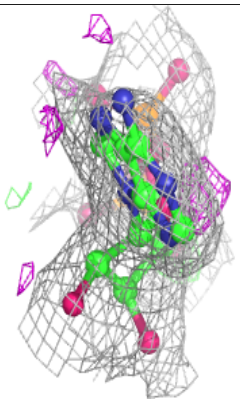


Electron density around ADP E 602:

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

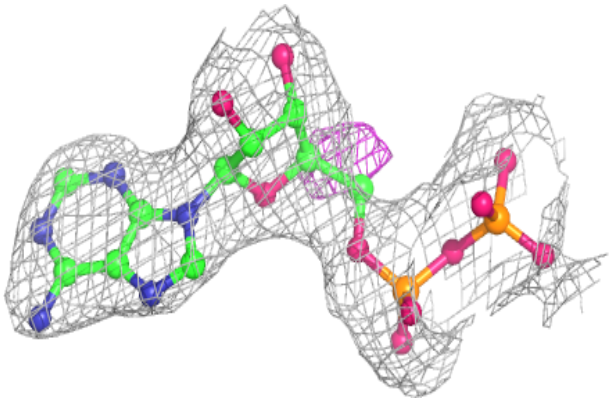


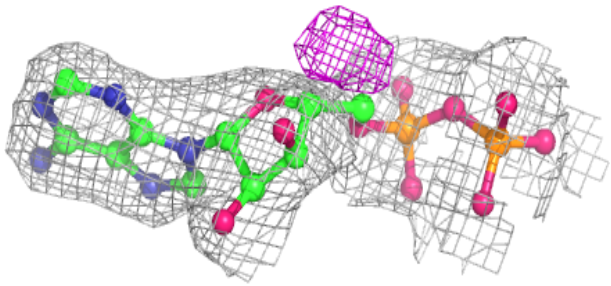


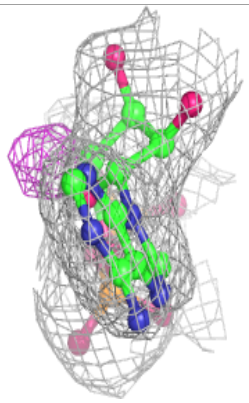


Electron density around ADP G 602:

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

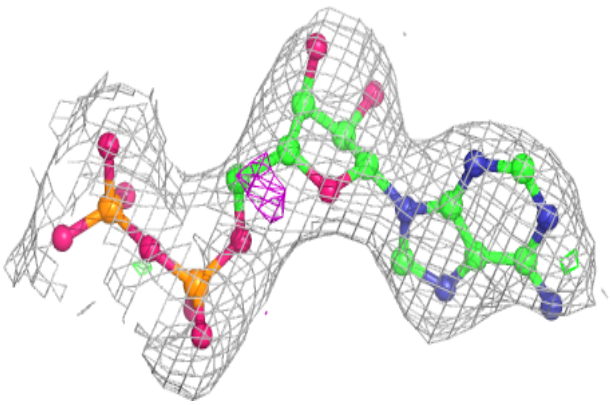


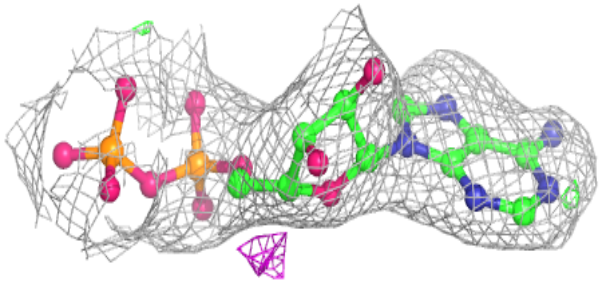


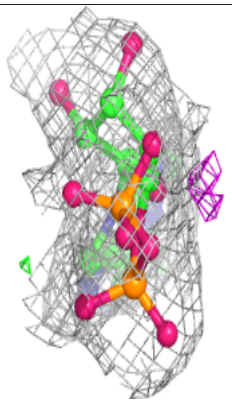


Electron density around ADP B 602:

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

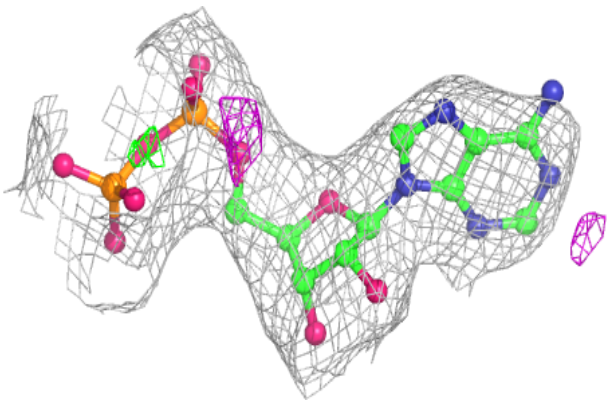


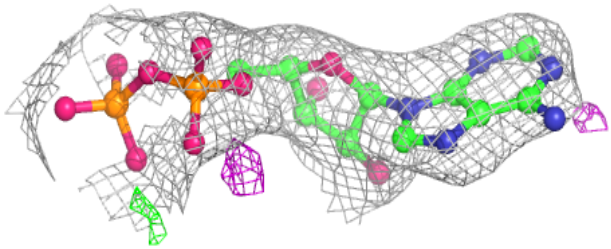


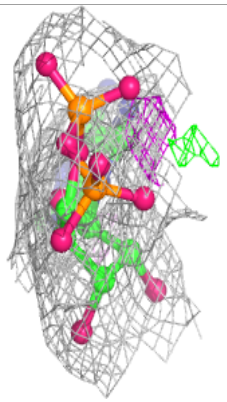


Electron density around ADP b 602:

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

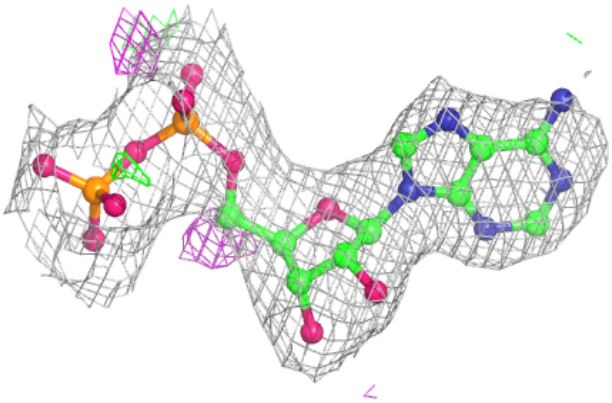


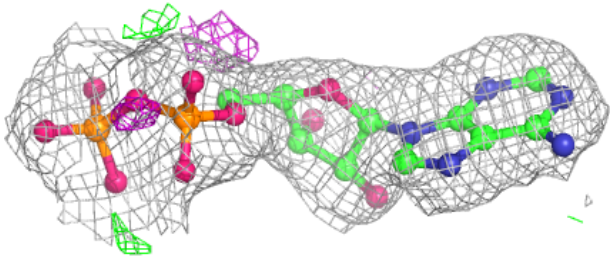


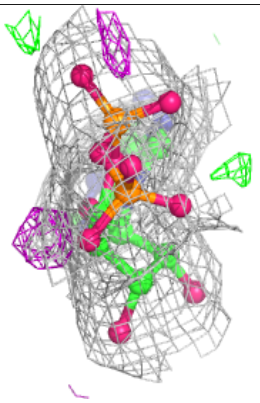


Electron density around ADP A 602:

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

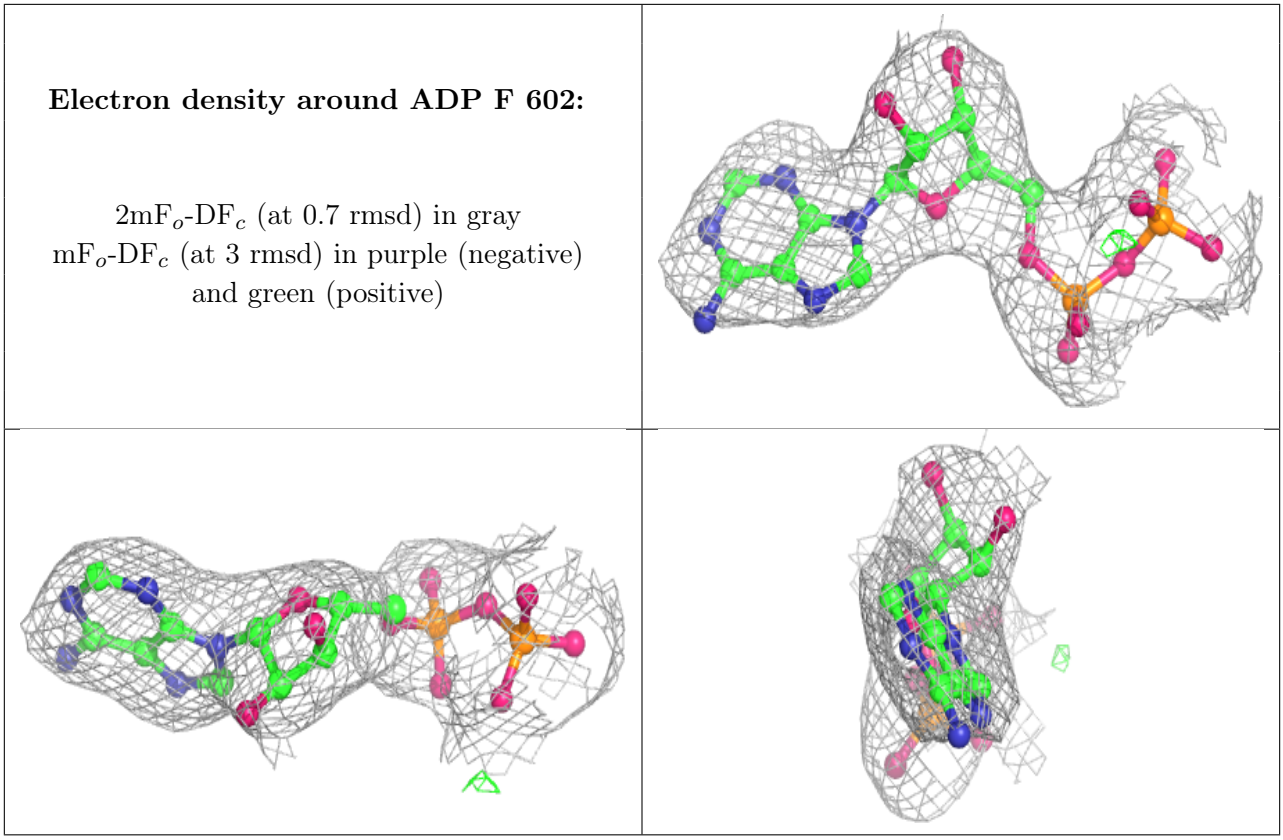






Electron density around ADP F 602:

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



6.5 Other polymers (i)

There are no such residues in this entry.