



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:24 AM GMT

PDB ID : 3OAA  
Title : Structure of the E.coli F1-ATP synthase inhibited by subunit Epsilon  
Authors : Cingolani, G.; Duncan, T.M.  
Deposited on : 2010-08-05  
Resolution : 3.26 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

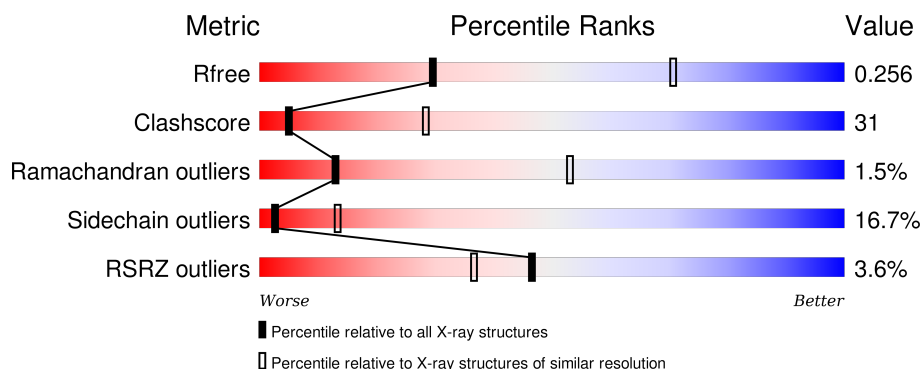
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.26 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))
$R_{free}$	91344	1624 (3.32-3.20)
Clashscore	102246	1806 (3.32-3.20)
Ramachandran outliers	100387	1773 (3.32-3.20)
Sidechain outliers	100360	1771 (3.32-3.20)
RSRZ outliers	91569	1632 (3.32-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	513	<div> <div></div> <div> <div>34%</div> <div>50%</div> <div>11%</div> <div>5%</div> </div> </div>
1	B	513	<div> <div>2%</div> <div> <div>47%</div> <div>37%</div> <div>10%</div> <div>5%</div> </div> </div>
1	C	513	<div> <div>0%</div> <div> <div>44%</div> <div>41%</div> <div>9%</div> <div>5%</div> </div> </div>
1	I	513	<div> <div>2%</div> <div> <div>49%</div> <div>37%</div> <div>9%</div> <div>5%</div> </div> </div>
1	J	513	<div> <div>3%</div> <div> <div>47%</div> <div>38%</div> <div>10%</div> <div>5%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	K	513	
1	Q	513	
1	R	513	
1	S	513	
1	Y	513	
1	Z	513	
1	a	513	
2	D	459	
2	E	459	
2	F	459	
2	L	459	
2	M	459	
2	N	459	
2	T	459	
2	U	459	
2	V	459	
2	b	459	
2	c	459	
2	d	459	
3	G	286	
3	O	286	
3	W	286	
3	e	286	
4	H	138	
4	P	138	

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Mol	Chain	Length	Quality of chain
4	X	138	
4	f	138	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	SO4	G	300	-	-	-	X
8	SO4	H	200	-	-	-	X
8	SO4	O	300	-	-	-	X
8	SO4	P	200	-	-	-	X
8	SO4	W	300	-	-	-	X

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 99573 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP synthase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	488	Total	C	N	O	S	0	0	0
			3667	2301	648	705	13			
1	B	486	Total	C	N	O	S	0	0	0
			3627	2278	642	694	13			
1	C	487	Total	C	N	O	S	0	0	0
			3646	2288	646	699	13			
1	I	488	Total	C	N	O	S	0	0	0
			3667	2301	648	705	13			
1	J	486	Total	C	N	O	S	0	0	0
			3627	2278	642	694	13			
1	K	487	Total	C	N	O	S	0	0	0
			3646	2288	646	699	13			
1	Q	488	Total	C	N	O	S	0	0	0
			3667	2301	648	705	13			
1	R	486	Total	C	N	O	S	0	0	0
			3627	2278	642	694	13			
1	S	487	Total	C	N	O	S	0	0	0
			3646	2288	646	699	13			
1	Y	488	Total	C	N	O	S	0	0	0
			3667	2301	648	705	13			
1	Z	486	Total	C	N	O	S	0	0	0
			3627	2278	642	694	13			
1	a	487	Total	C	N	O	S	0	0	0
			3646	2288	646	699	13			

- Molecule 2 is a protein called ATP synthase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	E	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	F	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	L	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	M	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	N	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	T	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	U	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	V	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	b	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	c	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			
2	d	458	Total	C	N	O	S	0	0	0
			3521	2218	601	687	15			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
E	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
F	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
L	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
M	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
N	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
T	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
U	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
V	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
b	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
c	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4
d	81	GLU	LYS	ENGINEERED MUTATION	UNP C9QXA4

- Molecule 3 is a protein called ATP synthase gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	284	Total	C	N	O	S	0	0	0
			2182	1369	382	417	14			

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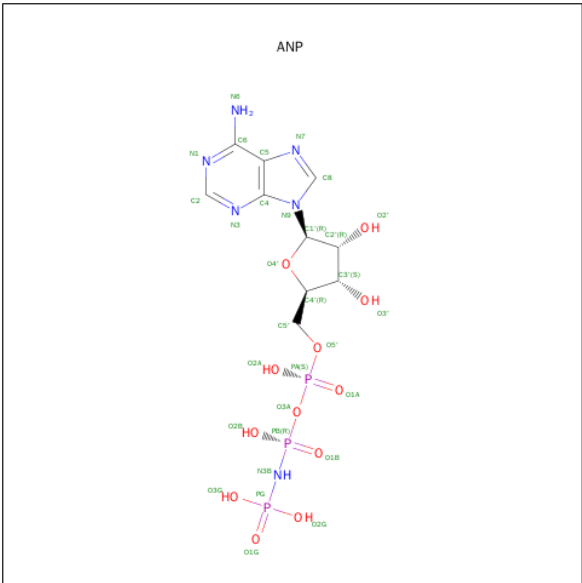
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	O	284	Total	C	N	O	S	0	0	0
			2182	1369	382	417	14			
3	W	284	Total	C	N	O	S	0	0	0
			2182	1369	382	417	14			
3	e	284	Total	C	N	O	S	0	0	0
			2182	1369	382	417	14			

- Molecule 4 is a protein called ATP synthase epsilon chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	138	Total	C	N	O	S	0	0	0
			1047	657	182	203	5			
4	P	138	Total	C	N	O	S	0	0	0
			1047	657	182	203	5			
4	X	138	Total	C	N	O	S	0	0	0
			1047	657	182	203	5			
4	f	138	Total	C	N	O	S	0	0	0
			1047	657	182	203	5			

- Molecule 5 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	I	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	K	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	Q	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	R	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	S	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	Y	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	Z	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
5	a	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total	Mg	0	0
			1	1		
6	Q	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		
6	K	1	Total	Mg	0	0
			1	1		
6	b	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	I	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	a	1	Total	Mg	0	0
			1	1		

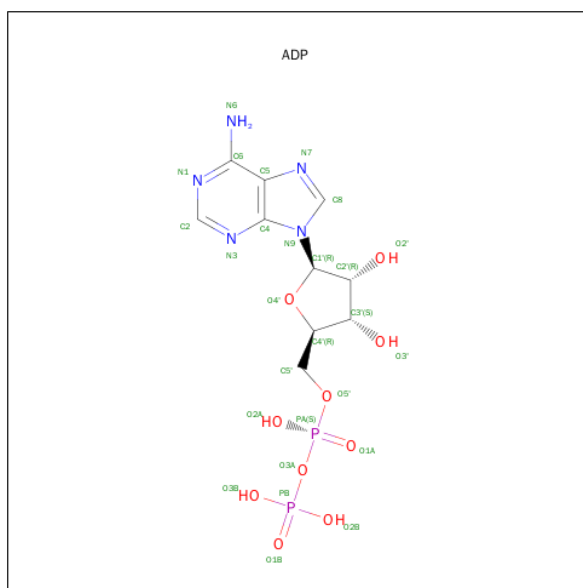
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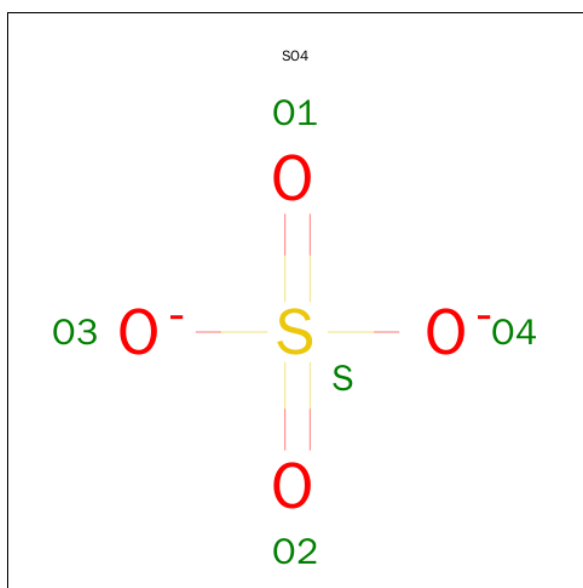
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	Z	1	Total	Mg	0	0
			1	1		
6	A	1	Total	Mg	0	0
			1	1		
6	T	1	Total	Mg	0	0
			1	1		
6	R	1	Total	Mg	0	0
			1	1		
6	Y	1	Total	Mg	0	0
			1	1		
6	L	1	Total	Mg	0	0
			1	1		
6	S	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	L	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	T	1	Total 27	C 10	N 5	O 10	P 2	0	0
7	b	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 8 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	O	S	0	0
			5	4	1		
8	E	1	Total	O	S	0	0
			5	4	1		
8	F	1	Total	O	S	0	0
			5	4	1		
8	G	1	Total	O	S	0	0
			5	4	1		
8	H	1	Total	O	S	0	0
			5	4	1		
8	L	1	Total	O	S	0	0
			5	4	1		
8	M	1	Total	O	S	0	0
			5	4	1		
8	N	1	Total	O	S	0	0
			5	4	1		
8	O	1	Total	O	S	0	0
			5	4	1		
8	P	1	Total	O	S	0	0
			5	4	1		
8	T	1	Total	O	S	0	0
			5	4	1		
8	U	1	Total	O	S	0	0
			5	4	1		
8	V	1	Total	O	S	0	0
			5	4	1		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	W	1	Total	O	S	0	0
			5	4	1		
8	b	1	Total	O	S	0	0
			5	4	1		
8	c	1	Total	O	S	0	0
			5	4	1		
8	d	1	Total	O	S	0	0
			5	4	1		

- Molecule 9 is water.

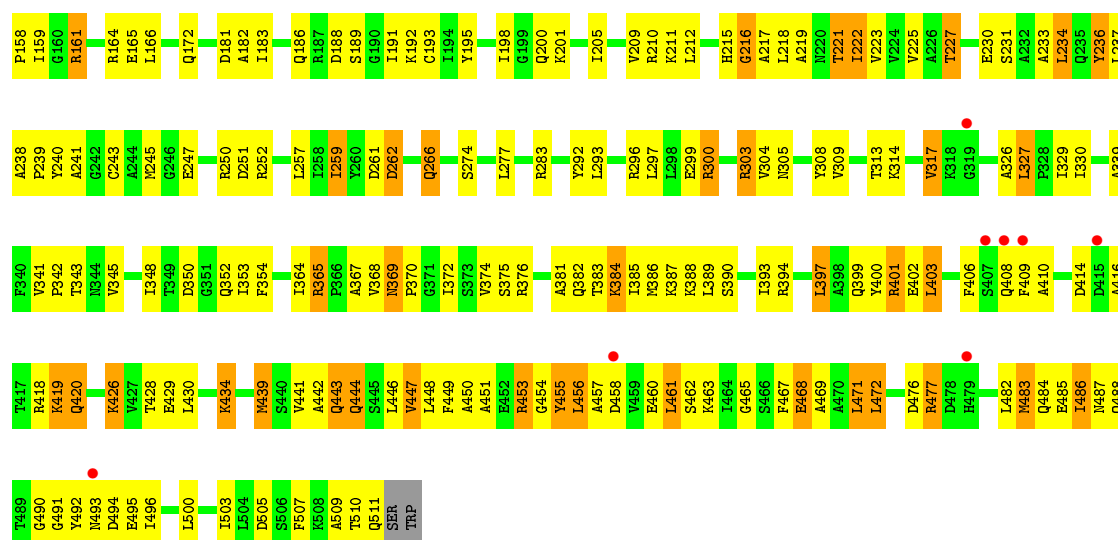
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	3	Total	O	0	0
			3	3		
9	B	2	Total	O	0	0
			2	2		
9	C	2	Total	O	0	0
			2	2		
9	D	8	Total	O	0	0
			8	8		
9	E	1	Total	O	0	0
			1	1		
9	F	5	Total	O	0	0
			5	5		
9	G	10	Total	O	0	0
			10	10		
9	H	4	Total	O	0	0
			4	4		
9	J	3	Total	O	0	0
			3	3		
9	L	6	Total	O	0	0
			6	6		
9	N	3	Total	O	0	0
			3	3		
9	O	5	Total	O	0	0
			5	5		
9	P	2	Total	O	0	0
			2	2		
9	Q	1	Total	O	0	0
			1	1		
9	R	1	Total	O	0	0
			1	1		

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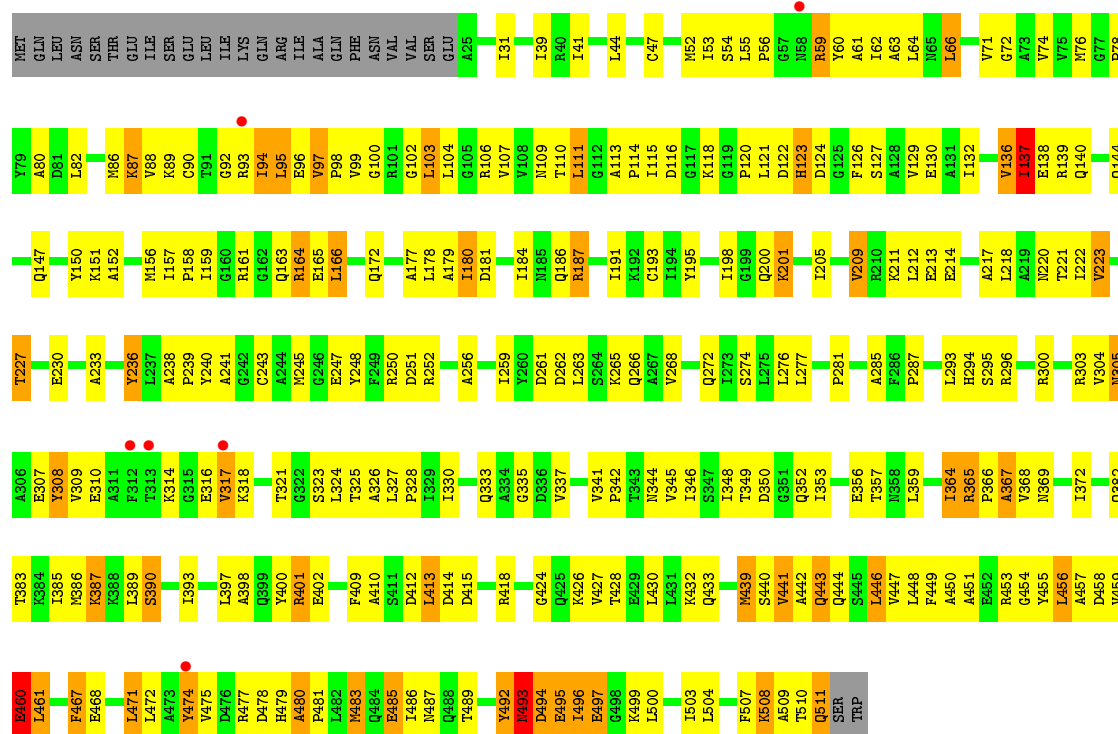
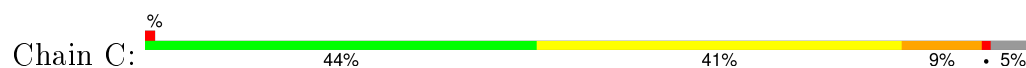
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	S	1	Total 1	O 1	0	0
9	V	2	Total 2	O 2	0	0
9	X	1	Total 1	O 1	0	0
9	a	1	Total 1	O 1	0	0
9	b	1	Total 1	O 1	0	0
9	d	2	Total 2	O 2	0	0

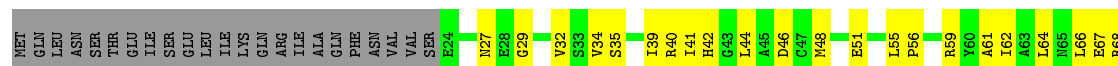


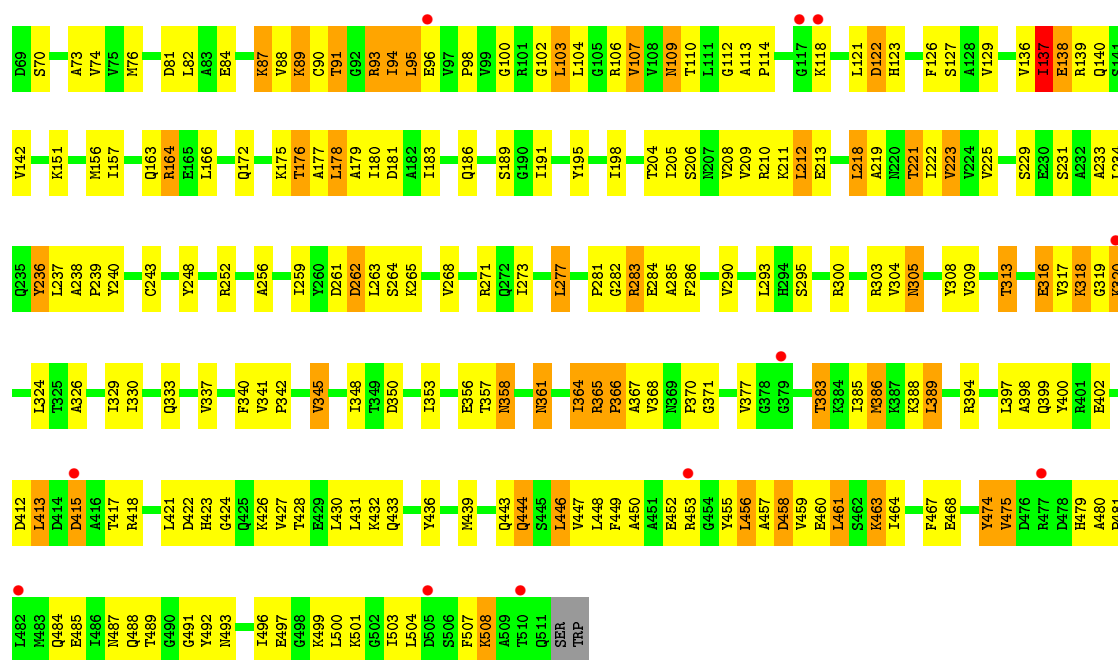


• Molecule 1: ATP synthase subunit alpha

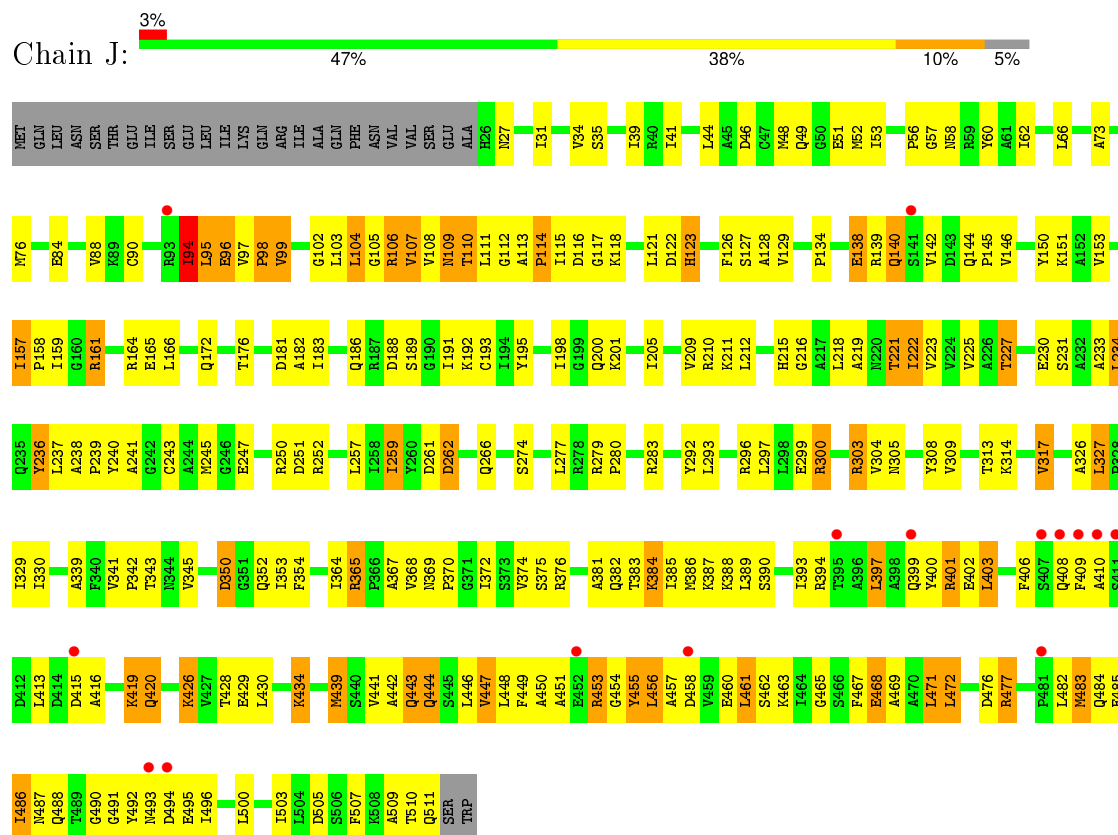


• Molecule 1: ATP synthase subunit alpha

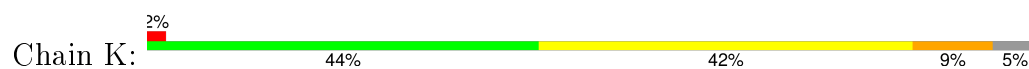


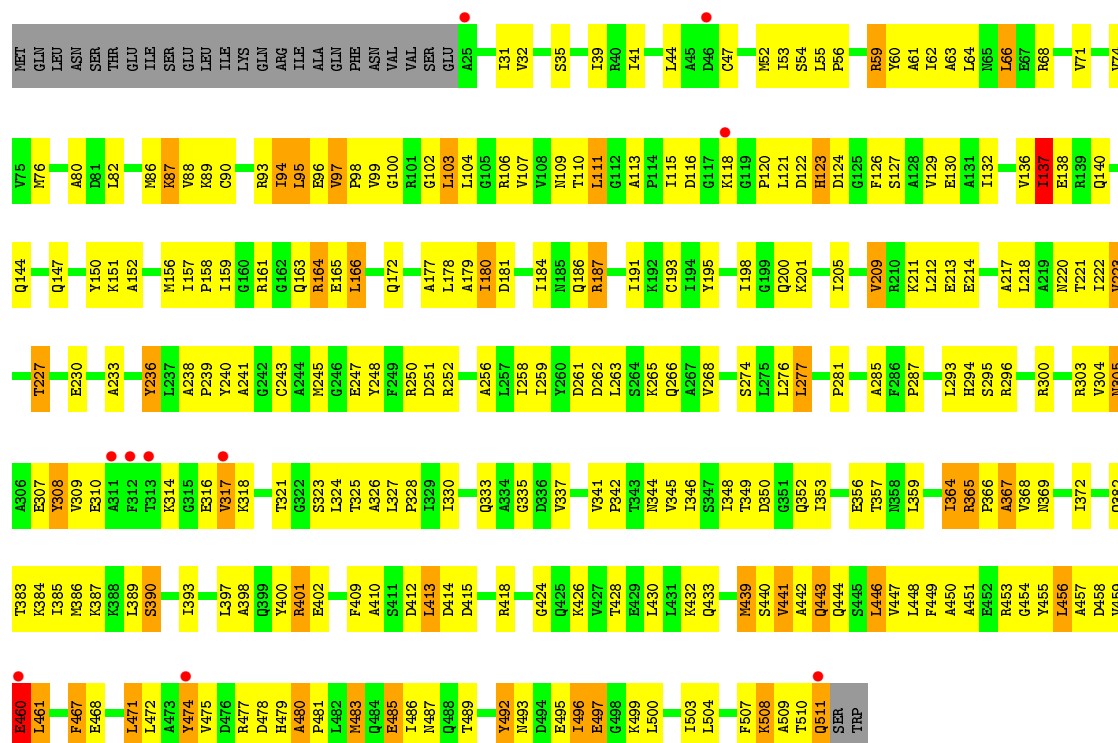


• Molecule 1: ATP synthase subunit alpha

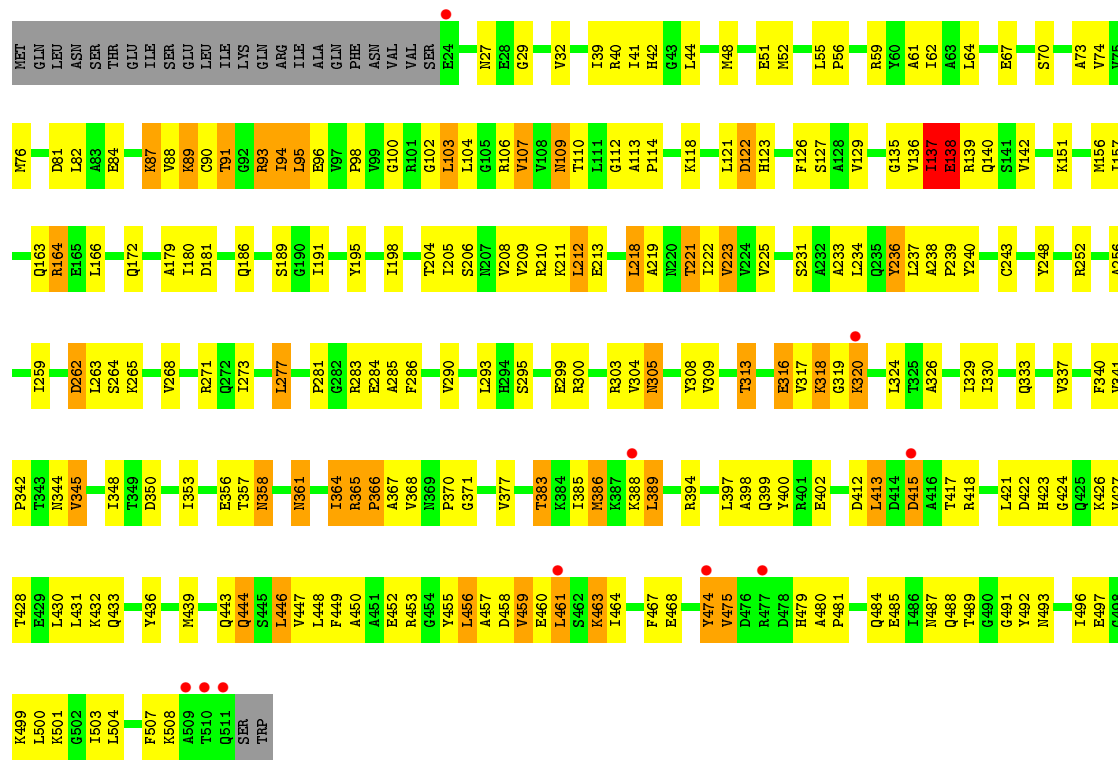


• Molecule 1: ATP synthase subunit alpha



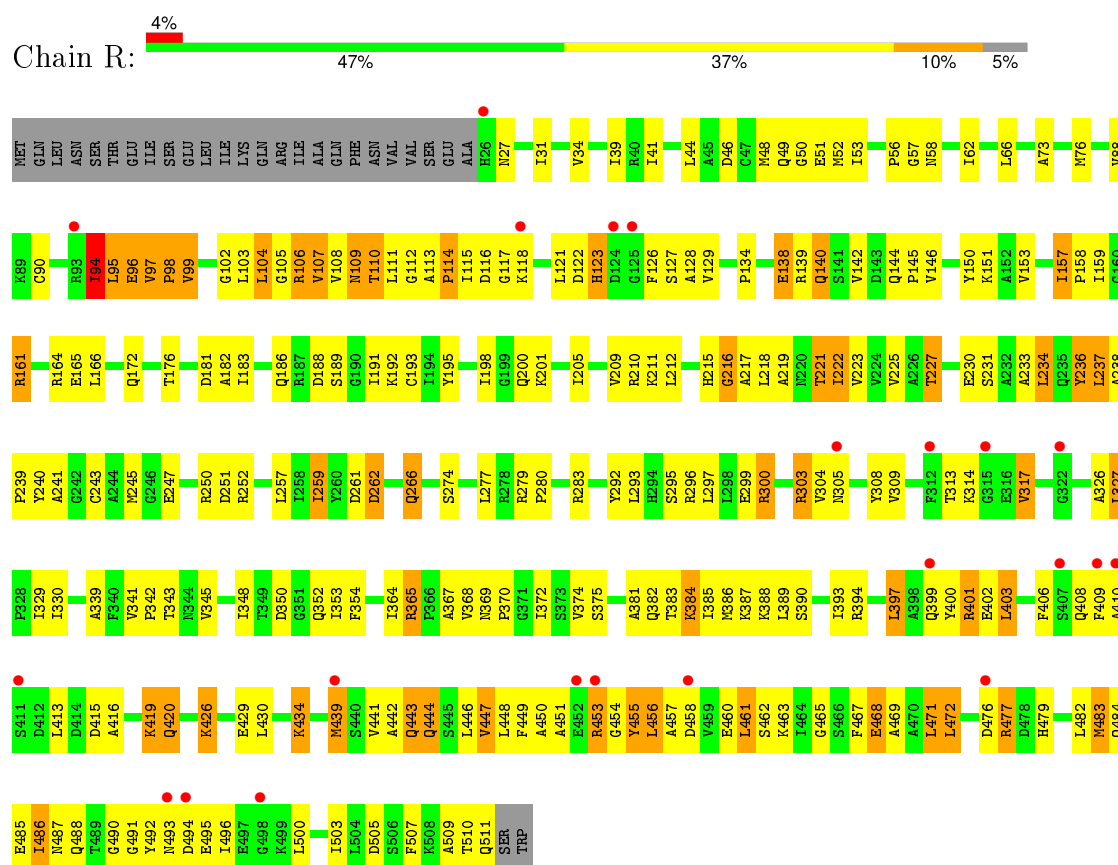


### • Molecule 1: ATP synthase subunit alpha

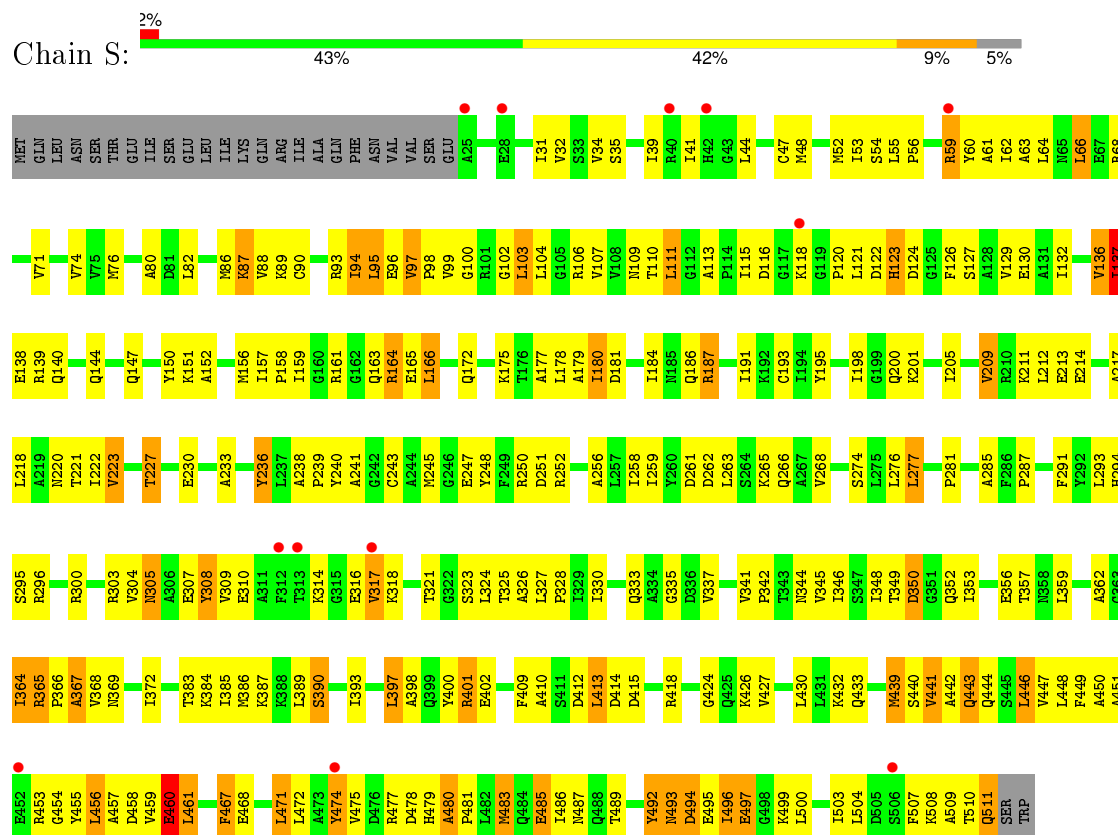


### • Molecule 1: ATP synthase subunit alpha

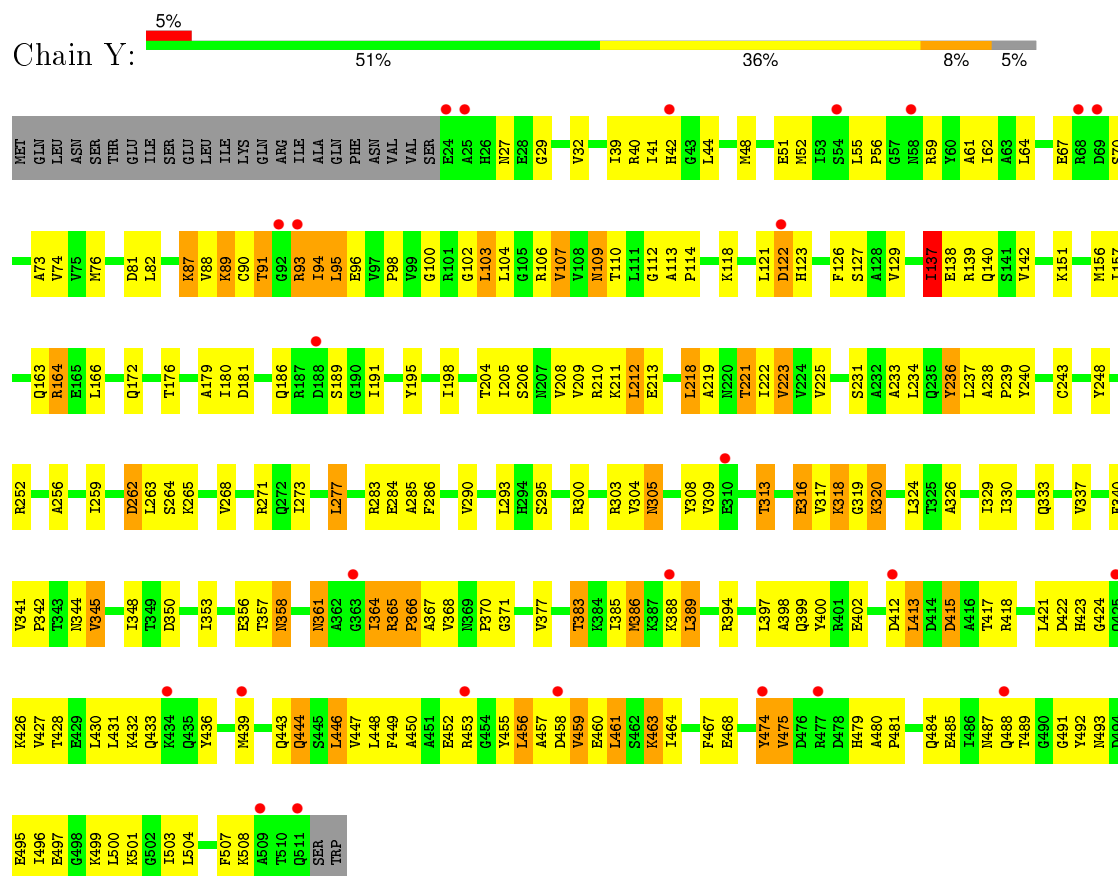




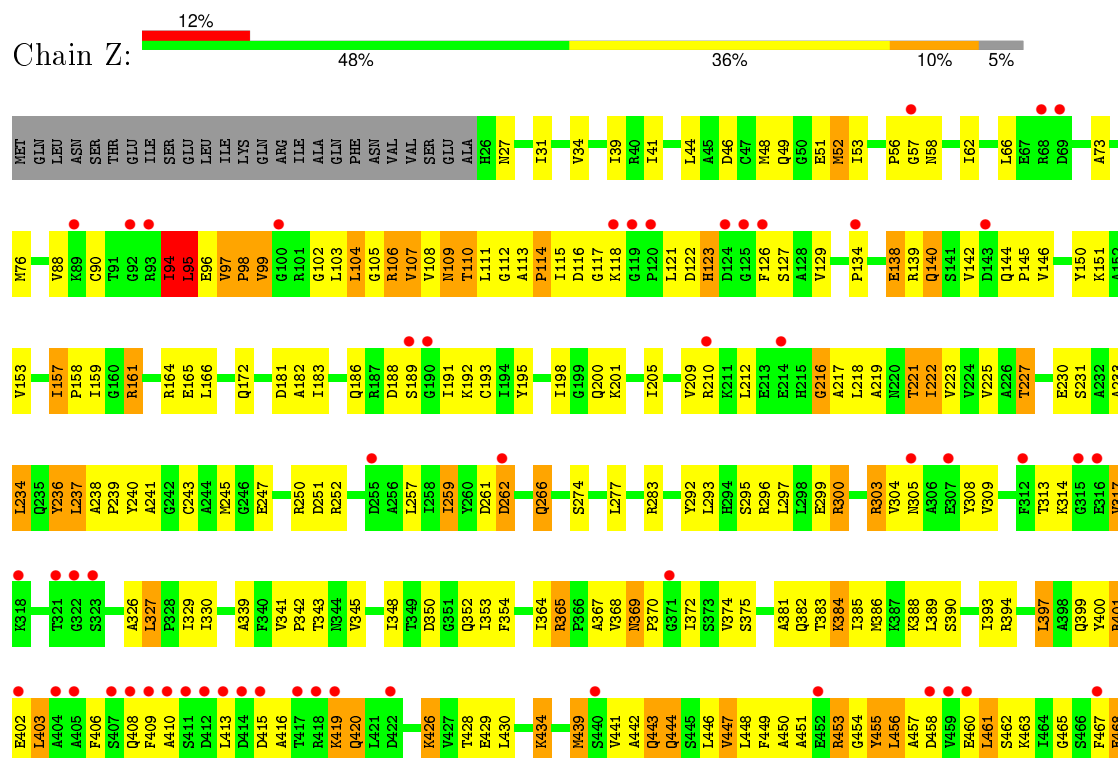
• Molecule 1: ATP synthase subunit alpha

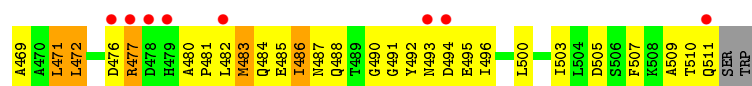


• Molecule 1: ATP synthase subunit alpha

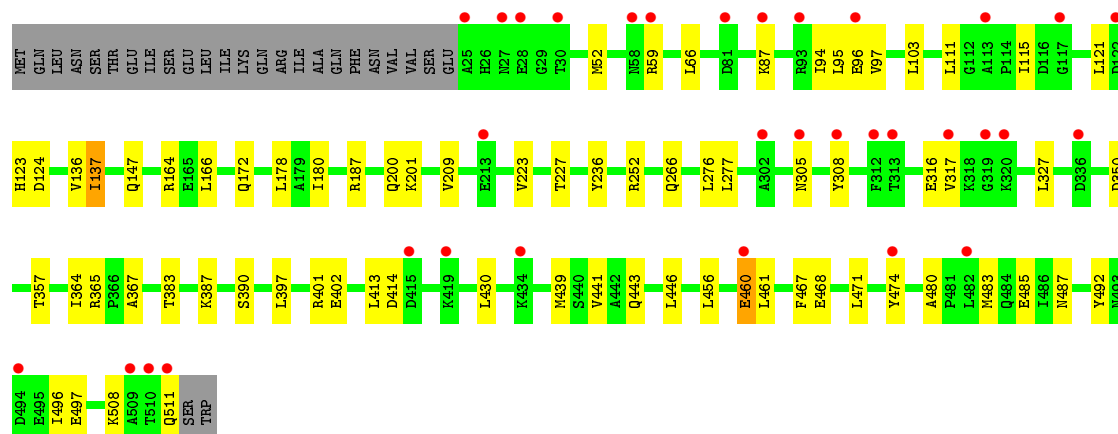
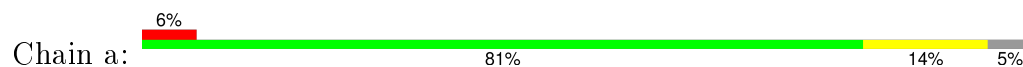


• Molecule 1: ATP synthase subunit alpha

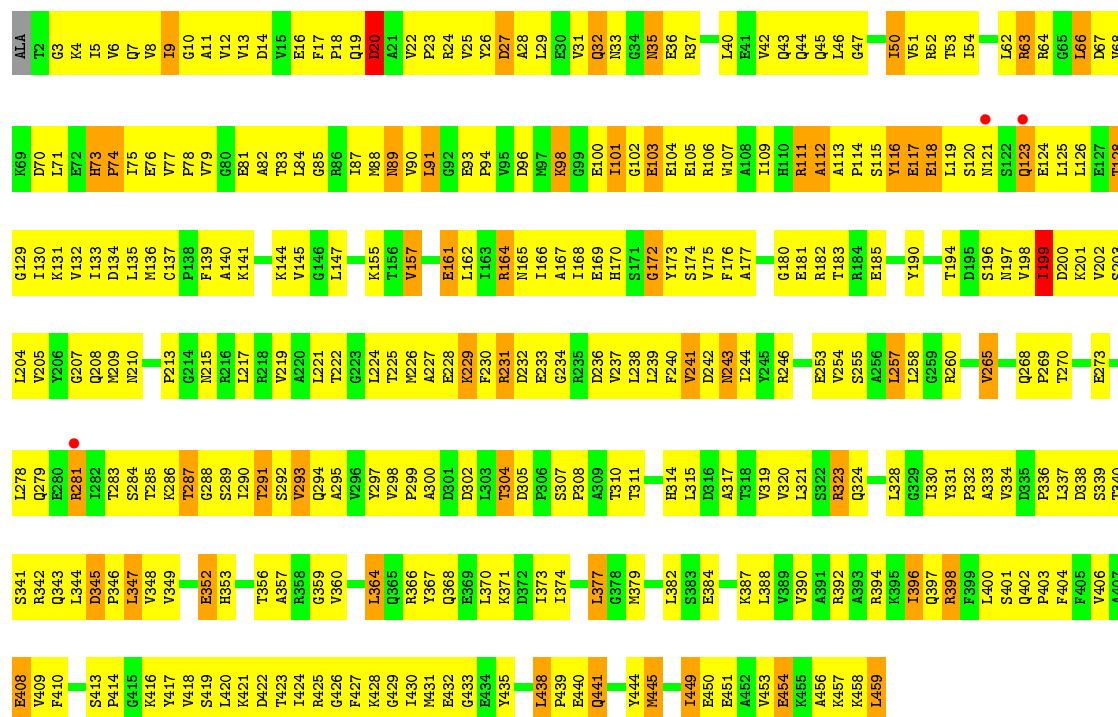




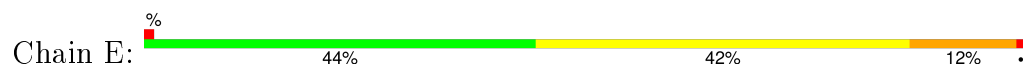
• Molecule 1: ATP synthase subunit alpha

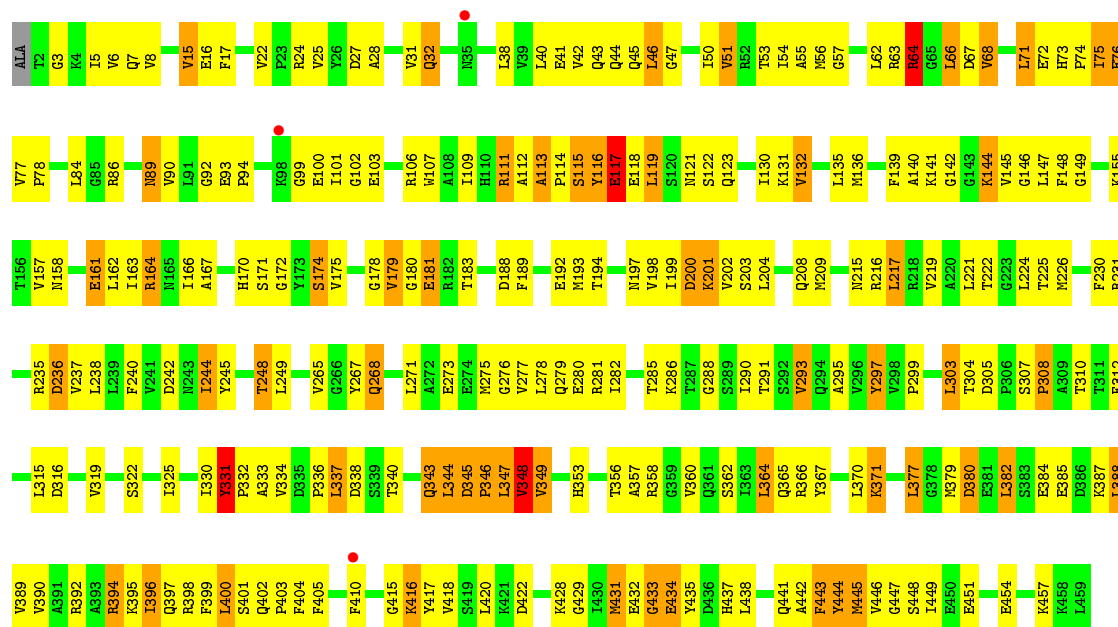


• Molecule 2: ATP synthase subunit beta

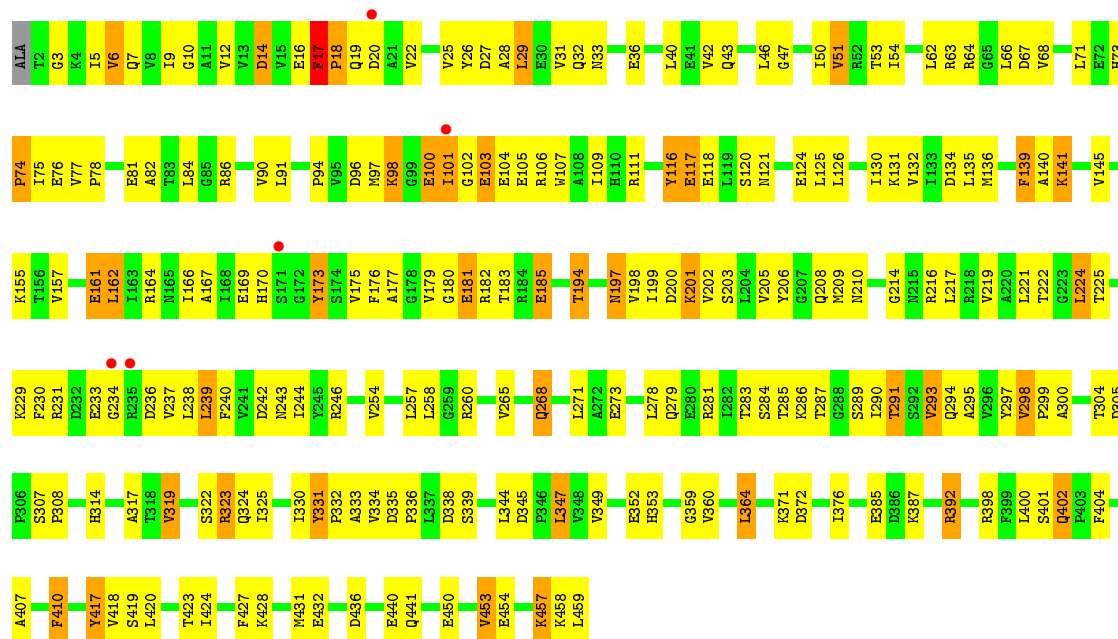


• Molecule 2: ATP synthase subunit beta

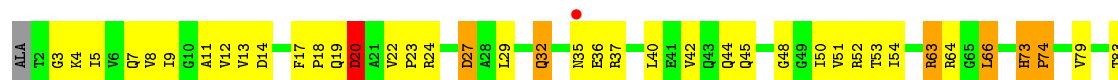


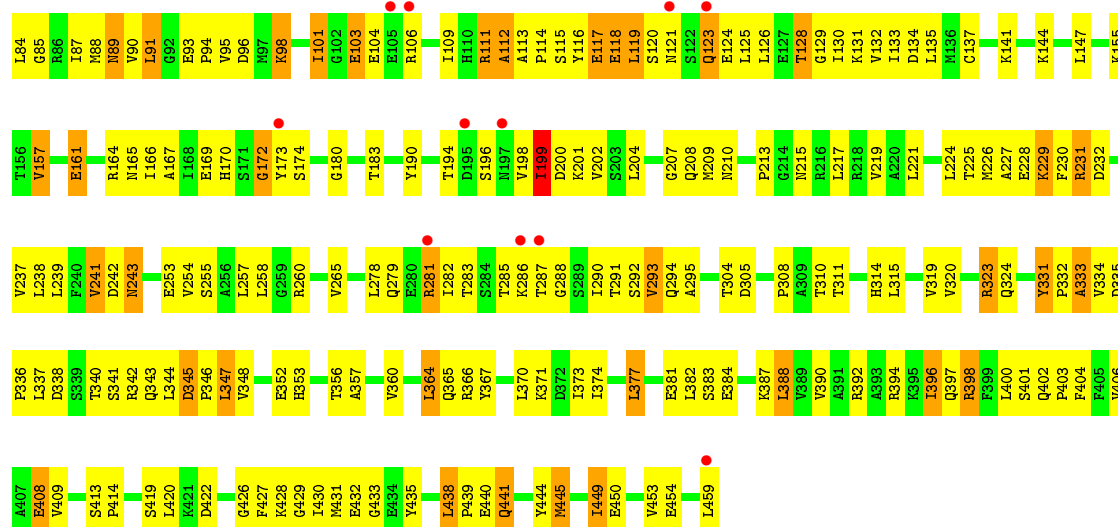


• Molecule 2: ATP synthase subunit beta

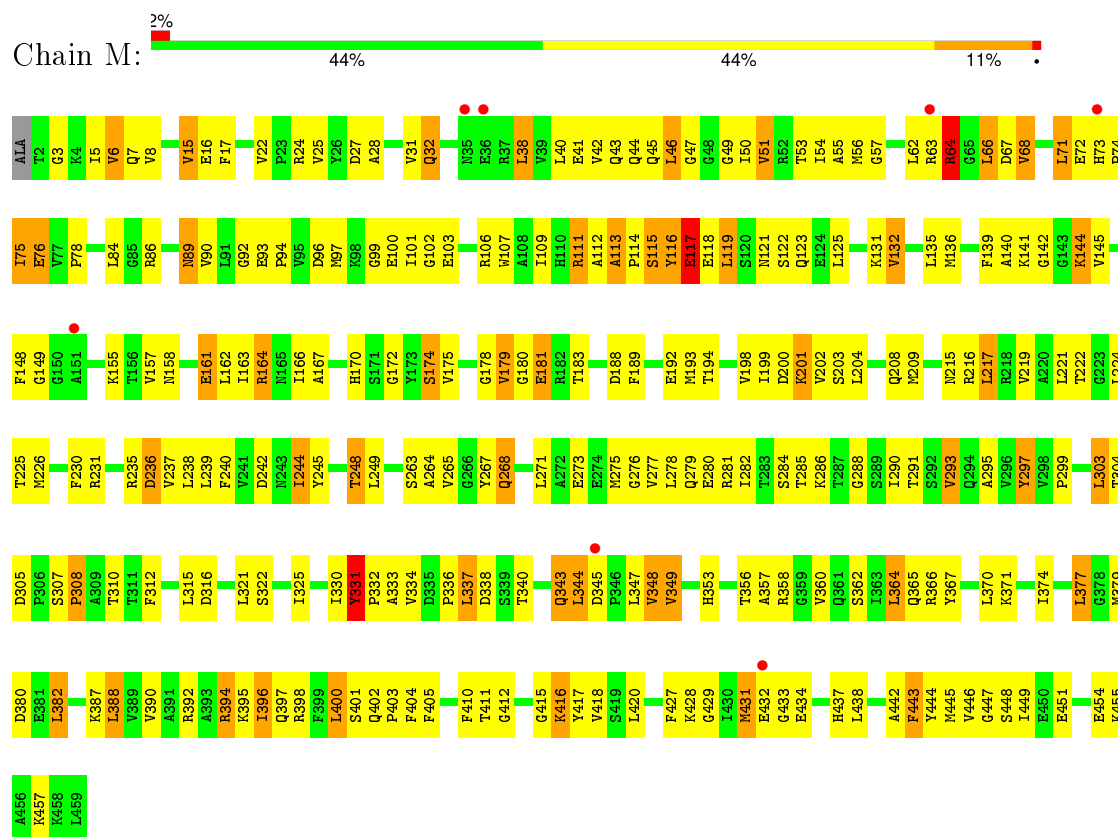


• Molecule 2: ATP synthase subunit beta

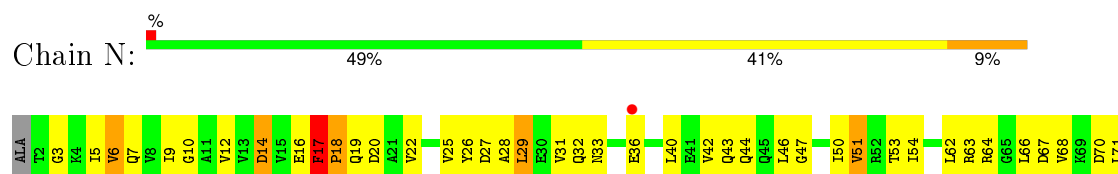


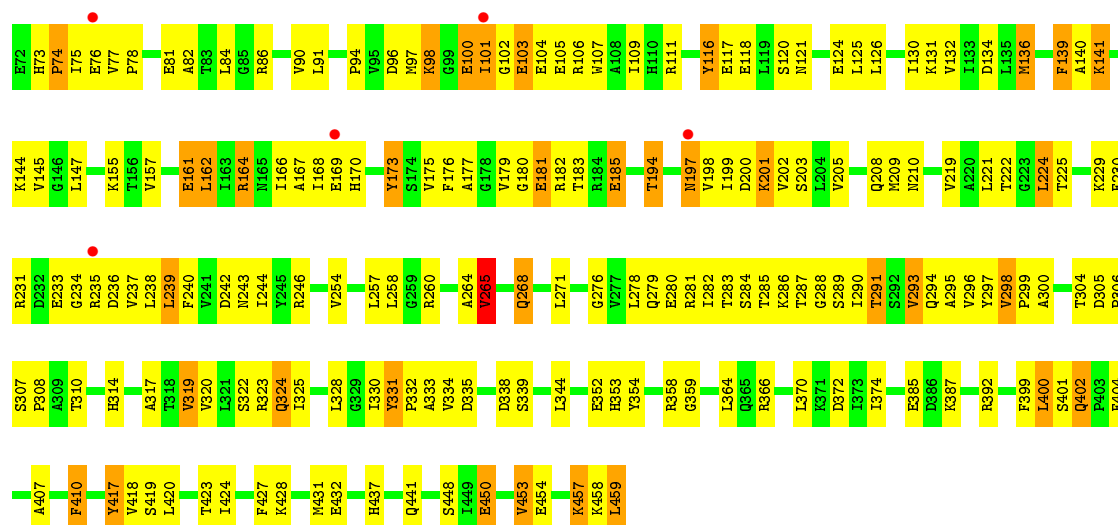


• Molecule 2: ATP synthase subunit beta

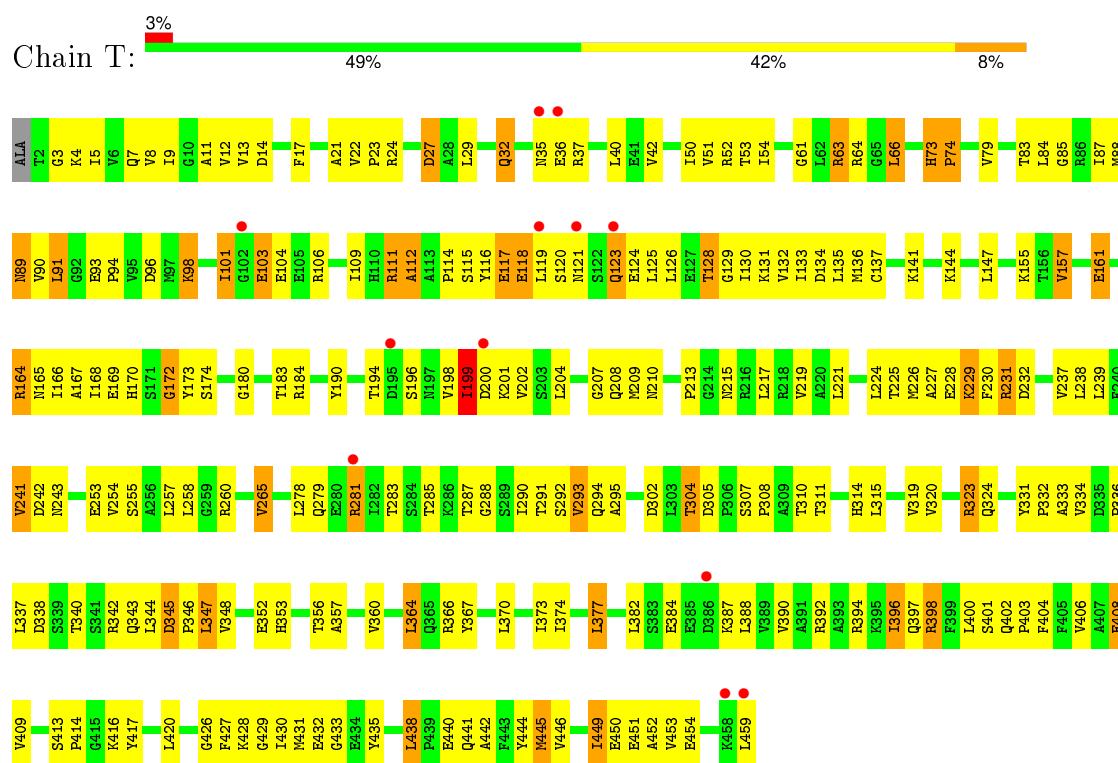


• Molecule 2: ATP synthase subunit beta

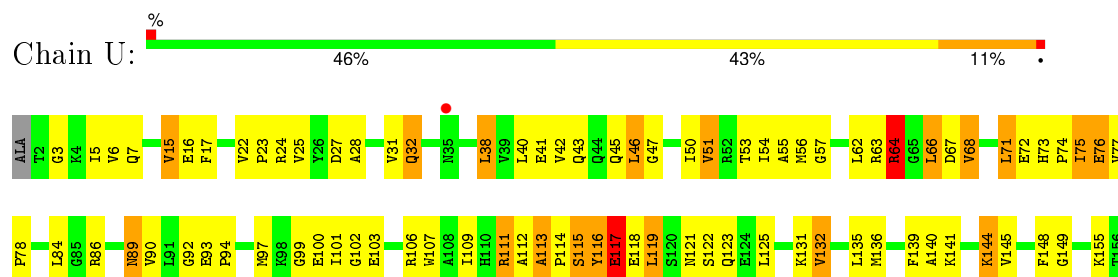


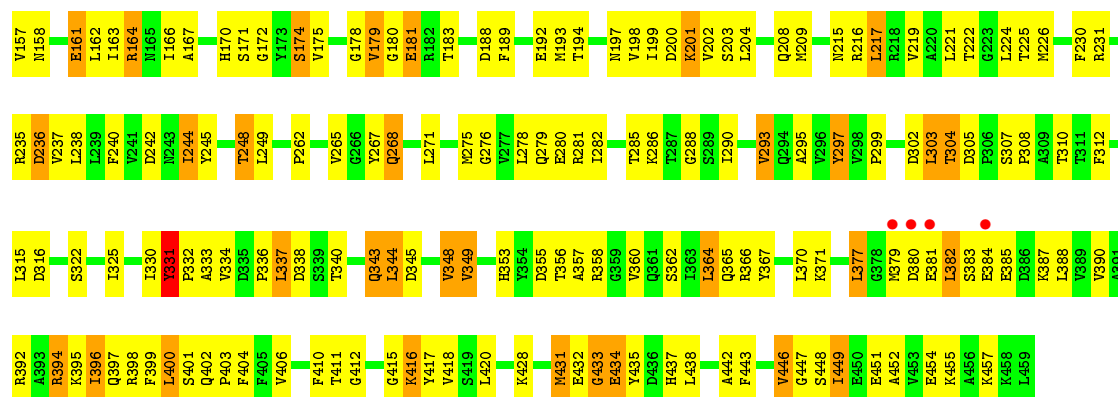


• Molecule 2: ATP synthase subunit beta

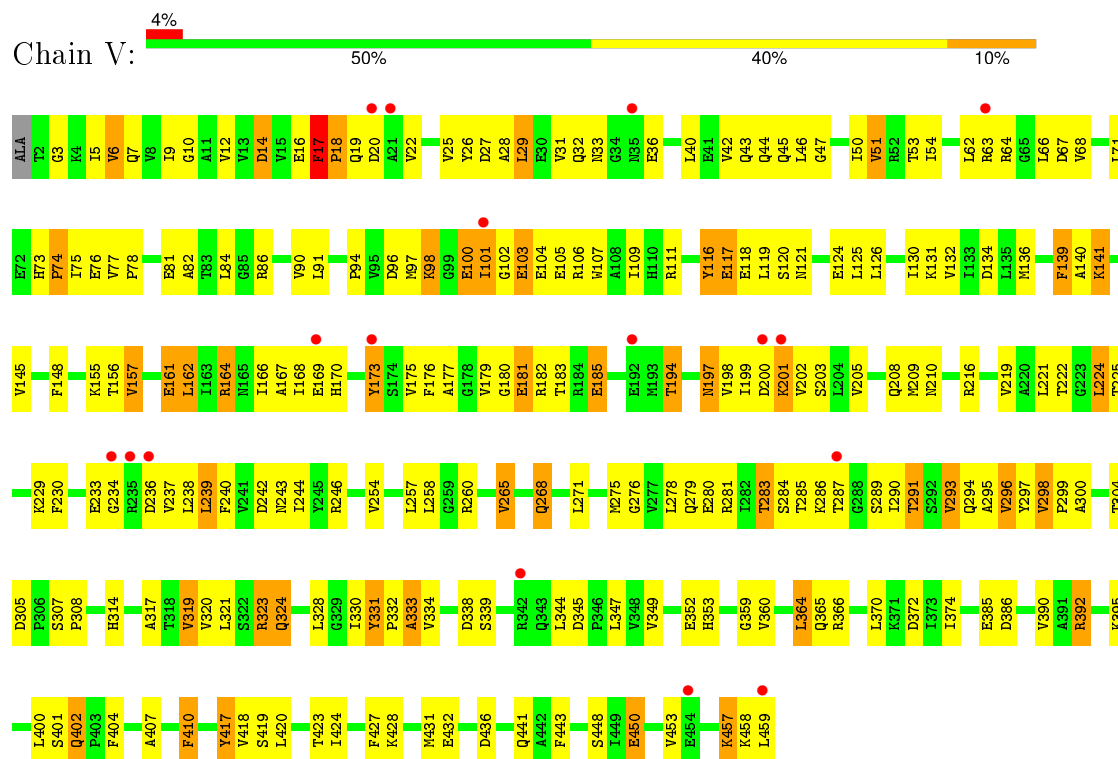


• Molecule 2: ATP synthase subunit beta

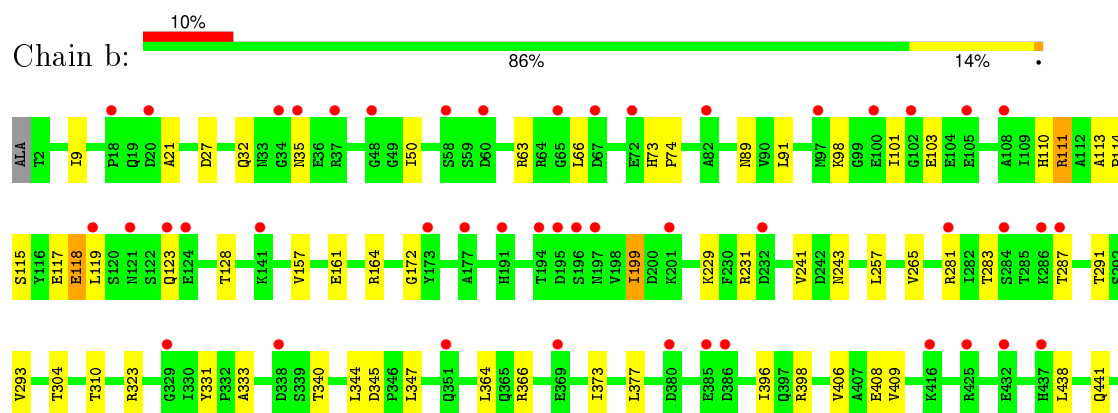


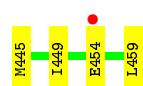


• Molecule 2: ATP synthase subunit beta

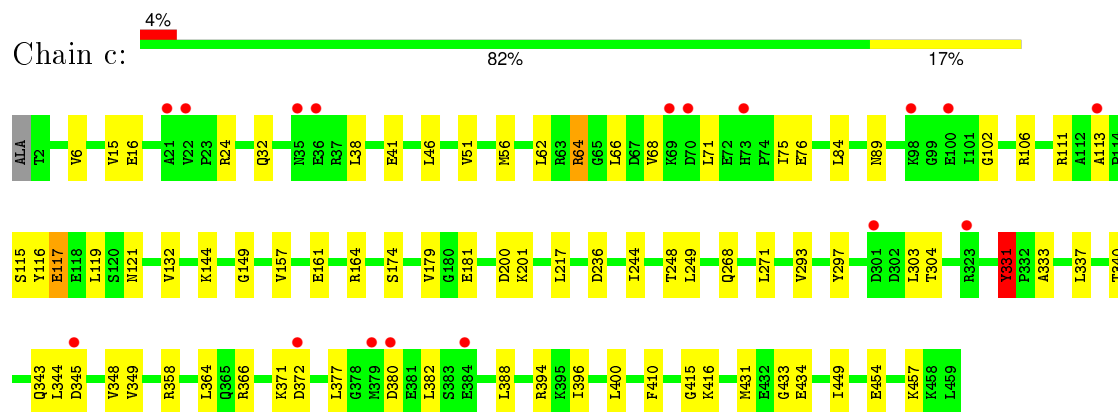


• Molecule 2: ATP synthase subunit beta

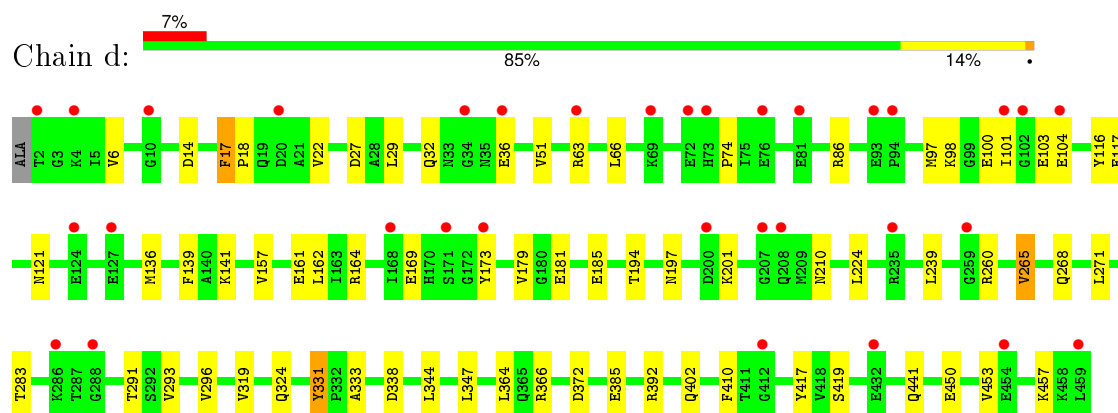




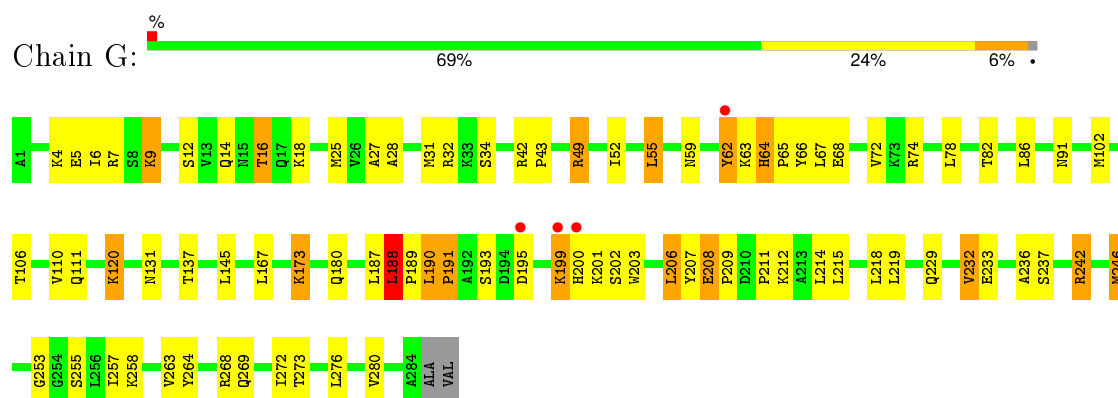
• Molecule 2: ATP synthase subunit beta



• Molecule 2: ATP synthase subunit beta



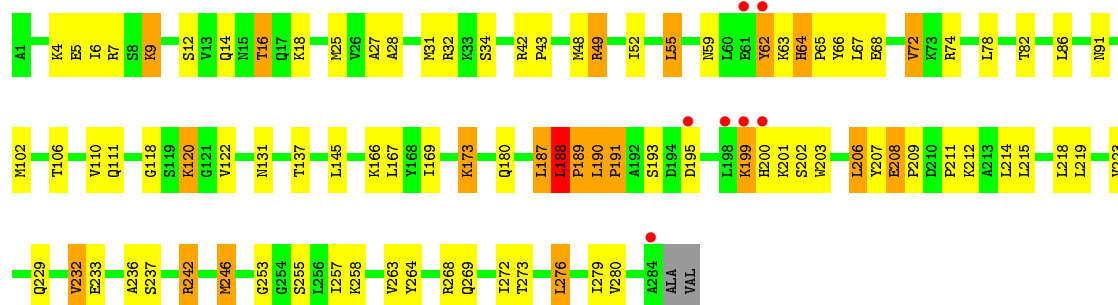
• Molecule 3: ATP synthase gamma chain



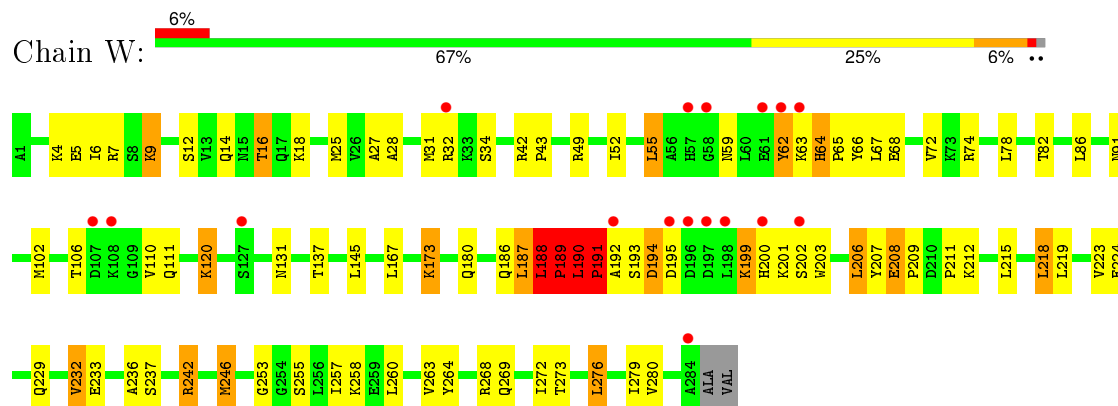
• Molecule 3: ATP synthase gamma chain



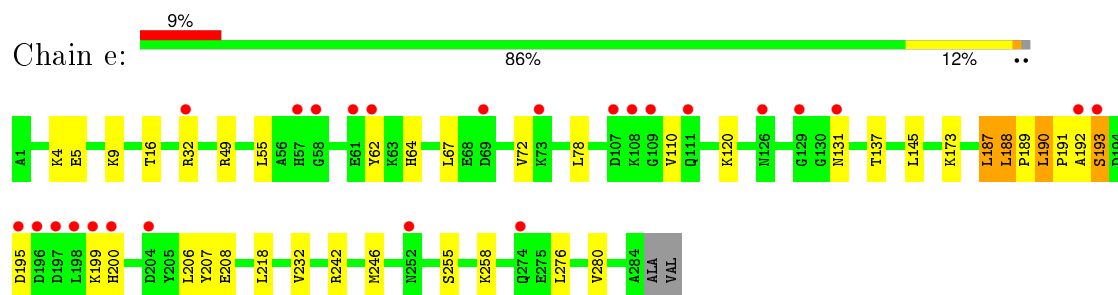




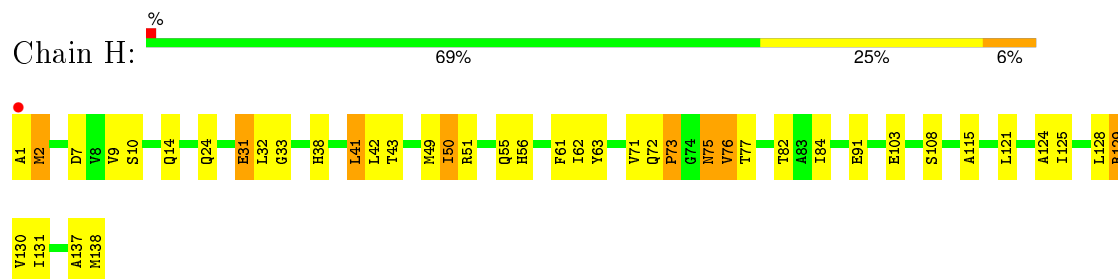
• Molecule 3: ATP synthase gamma chain



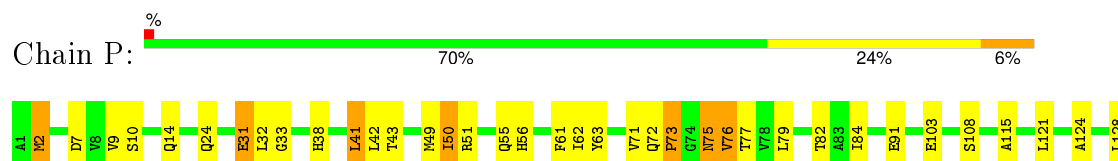
• Molecule 3: ATP synthase gamma chain



• Molecule 4: ATP synthase epsilon chain

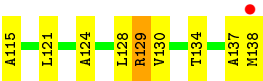
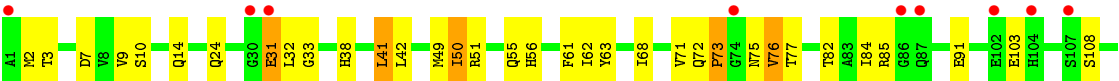


• Molecule 4: ATP synthase epsilon chain

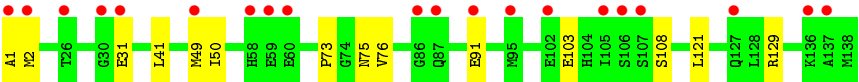
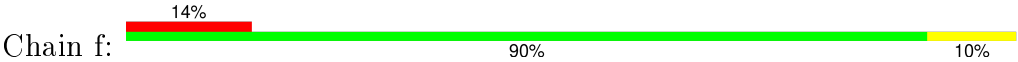




• Molecule 4: ATP synthase epsilon chain



• Molecule 4: ATP synthase epsilon chain



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	435.97Å 183.00Å 225.39Å 90.00° 108.99° 90.00°	Depositor
Resolution (Å)	15.00 – 3.26 15.11 – 3.26	Depositor EDS
% Data completeness (in resolution range)	98.0 (15.00-3.26) 98.0 (15.11-3.26)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.12 (at 3.26Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE: 1.6.3_473)	Depositor
R, $R_{free}$	0.243 , 0.265 0.233 , 0.256	Depositor DCC
$R_{free}$ test set	1993 reflections (0.79%)	DCC
Wilson B-factor (Å <sup>2</sup> )	79.5	Xtriage
Anisotropy	0.020	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.26 , 65.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 252343 reflections	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	99573	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ANP, SO4, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.27	0/3720	0.45	1/5032 (0.0%)
1	B	0.25	0/3679	0.48	1/4979 (0.0%)
1	C	0.24	0/3699	0.46	0/5005
1	I	0.28	0/3720	0.48	2/5032 (0.0%)
1	J	0.25	0/3679	0.48	1/4979 (0.0%)
1	K	0.24	0/3699	0.46	0/5005
1	Q	0.25	0/3720	0.45	1/5032 (0.0%)
1	R	0.25	0/3679	0.48	1/4979 (0.0%)
1	S	0.23	0/3699	0.46	0/5005
1	Y	0.22	0/3720	0.53	2/5032 (0.0%)
1	Z	0.25	0/3679	0.48	1/4979 (0.0%)
1	a	0.23	0/3699	0.46	0/5005
2	D	0.25	0/3578	0.47	1/4843 (0.0%)
2	E	0.28	0/3578	0.48	0/4843
2	F	0.23	0/3578	0.47	0/4843
2	L	0.24	0/3578	0.48	2/4843 (0.0%)
2	M	0.26	0/3578	0.48	0/4843
2	N	0.24	0/3578	0.48	0/4843
2	T	0.23	0/3578	0.50	3/4843 (0.1%)
2	U	0.26	0/3578	0.48	0/4843
2	V	0.23	0/3578	0.47	0/4843
2	b	0.25	0/3578	0.47	1/4843 (0.0%)
2	c	0.25	0/3578	0.47	0/4843
2	d	0.23	0/3578	0.46	0/4843
3	G	0.30	0/2213	0.46	1/2984 (0.0%)
3	O	0.28	0/2213	0.46	1/2984 (0.0%)
3	W	0.25	0/2213	0.44	1/2984 (0.0%)
3	e	0.24	0/2213	0.52	1/2984 (0.0%)
4	H	0.22	0/1062	0.85	2/1432 (0.1%)
4	P	0.22	0/1062	0.40	0/1432
4	X	0.22	0/1062	0.40	0/1432
4	f	0.23	0/1062	0.86	2/1432 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
All	All	0.25	0/100428	0.48	25/135844 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	2
1	I	1	1
1	J	0	1
1	K	0	1
1	Q	0	1
1	R	0	1
1	S	0	2
1	Y	1	1
1	Z	0	2
1	a	0	1
2	D	0	2
2	E	0	4
2	F	0	1
2	L	0	2
2	M	0	1
2	N	0	1
2	T	0	1
2	U	0	1
2	V	0	1
2	b	0	5
2	c	0	1
2	d	0	1
3	G	0	2
3	O	0	2
3	W	0	4
3	e	0	4
All	All	2	47

There are no bond length outliers.

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	1	ALA	CB-CA-C	27.46	151.29	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	f	1	ALA	CB-CA-C	27.44	151.26	110.10
1	Y	137	ILE	C-N-CA	-16.64	80.11	121.70
3	e	190	LEU	C-N-CD	-15.49	86.52	120.60
1	Y	137	ILE	N-CA-C	11.89	143.09	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	I	138	GLU	CA
1	Y	137	ILE	CA

5 of 47 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	135	GLY	Peptide
1	C	460	GLU	Peptide
1	C	493	ASN	Peptide
2	D	119	LEU	Peptide
2	D	20	ASP	Peptide

## 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	3667	0	3702	449	0
1	B	3627	0	3650	261	0
1	C	3646	0	3669	260	0
1	I	3667	0	3702	257	0
1	J	3627	0	3650	255	0
1	K	3646	0	3669	251	0
1	Q	3667	0	3702	225	0
1	R	3627	0	3650	267	0
1	S	3646	0	3669	256	0
1	Y	3667	0	3702	209	0
1	Z	3627	0	3650	248	0
1	a	3646	0	3669	0	0
2	D	3521	0	3523	448	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3521	0	3524	320	0
2	F	3521	0	3524	205	0
2	L	3521	0	3523	240	0
2	M	3521	0	3524	278	0
2	N	3521	0	3524	201	0
2	T	3521	0	3523	229	0
2	U	3521	0	3524	264	0
2	V	3521	0	3524	208	0
2	b	3521	0	3523	0	0
2	c	3521	0	3524	0	0
2	d	3521	0	3524	0	0
3	G	2182	0	2227	79	0
3	O	2182	0	2227	84	0
3	W	2182	0	2227	121	0
3	e	2182	0	2227	0	0
4	H	1047	0	1058	35	0
4	P	1047	0	1058	35	0
4	X	1047	0	1058	42	0
4	f	1047	0	1058	0	0
5	A	31	0	12	4	0
5	B	31	0	12	3	0
5	C	31	0	12	3	0
5	I	31	0	12	4	0
5	J	31	0	12	3	0
5	K	31	0	12	2	0
5	Q	31	0	12	2	0
5	R	31	0	12	3	0
5	S	31	0	12	2	0
5	Y	31	0	12	3	0
5	Z	31	0	12	3	0
5	a	31	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	I	1	0	0	0	0
6	J	1	0	0	0	0
6	K	1	0	0	0	0
6	L	1	0	0	0	0
6	Q	1	0	0	0	0
6	R	1	0	0	0	0
6	S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	T	1	0	0	0	0
6	Y	1	0	0	0	0
6	Z	1	0	0	0	0
6	a	1	0	0	0	0
6	b	1	0	0	0	0
7	D	27	0	11	5	0
7	L	27	0	11	5	0
7	T	27	0	11	4	0
7	b	27	0	11	0	0
8	D	5	0	0	1	0
8	E	5	0	0	0	0
8	F	5	0	0	1	0
8	G	5	0	0	0	0
8	H	5	0	0	0	0
8	L	5	0	0	1	0
8	M	5	0	0	0	0
8	N	5	0	0	1	0
8	O	5	0	0	0	0
8	P	5	0	0	0	0
8	T	5	0	0	0	0
8	U	5	0	0	0	0
8	V	5	0	0	0	0
8	W	5	0	0	1	0
8	b	5	0	0	0	0
8	c	5	0	0	0	0
8	d	5	0	0	0	0
9	A	3	0	0	0	0
9	B	2	0	0	0	0
9	C	2	0	0	0	0
9	D	8	0	0	0	0
9	E	1	0	0	0	0
9	F	5	0	0	0	0
9	G	10	0	0	0	0
9	H	4	0	0	0	0
9	J	3	0	0	0	0
9	L	6	0	0	0	0
9	N	3	0	0	0	0
9	O	5	0	0	0	0
9	P	2	0	0	0	0
9	Q	1	0	0	0	0
9	R	1	0	0	0	0
9	S	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	V	2	0	0	0	0
9	X	1	0	0	0	0
9	a	1	0	0	0	0
9	b	1	0	0	0	0
9	d	2	0	0	0	0
All	All	99573	0	99696	5529	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 31.

The worst 5 of 5529 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ILE:HD13	1:A:138:GLU:CA	1.35	1.50
1:R:50:GLY:O	1:R:94:ILE:CG2	1.63	1.45
3:W:186:GLN:NE2	3:W:189:PRO:HG2	1.31	1.45
1:R:95:LEU:CD2	1:R:129:VAL:HG22	1.44	1.42
1:Y:137:ILE:CD1	1:Y:137:ILE:O	1.69	1.39

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	486/513 (95%)	433 (89%)	48 (10%)	5 (1%)	19	62
1	B	484/513 (94%)	421 (87%)	54 (11%)	9 (2%)	10	48
1	C	485/513 (94%)	429 (88%)	48 (10%)	8 (2%)	12	52
1	I	486/513 (95%)	433 (89%)	49 (10%)	4 (1%)	24	66
1	J	484/513 (94%)	419 (87%)	56 (12%)	9 (2%)	10	48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	485/513 (94%)	428 (88%)	49 (10%)	8 (2%)	12	52
1	Q	486/513 (95%)	433 (89%)	47 (10%)	6 (1%)	16	58
1	R	484/513 (94%)	417 (86%)	58 (12%)	9 (2%)	10	48
1	S	485/513 (94%)	429 (88%)	48 (10%)	8 (2%)	12	52
1	Y	486/513 (95%)	431 (89%)	49 (10%)	6 (1%)	16	58
1	Z	484/513 (94%)	418 (86%)	57 (12%)	9 (2%)	10	48
1	a	485/513 (94%)	427 (88%)	50 (10%)	8 (2%)	12	52
2	D	456/459 (99%)	397 (87%)	54 (12%)	5 (1%)	17	60
2	E	456/459 (99%)	406 (89%)	38 (8%)	12 (3%)	7	39
2	F	456/459 (99%)	411 (90%)	40 (9%)	5 (1%)	17	60
2	L	456/459 (99%)	398 (87%)	53 (12%)	5 (1%)	17	60
2	M	456/459 (99%)	405 (89%)	41 (9%)	10 (2%)	8	43
2	N	456/459 (99%)	413 (91%)	37 (8%)	6 (1%)	15	56
2	T	456/459 (99%)	402 (88%)	48 (10%)	6 (1%)	15	56
2	U	456/459 (99%)	406 (89%)	38 (8%)	12 (3%)	7	39
2	V	456/459 (99%)	410 (90%)	40 (9%)	6 (1%)	15	56
2	b	456/459 (99%)	398 (87%)	51 (11%)	7 (2%)	13	53
2	c	456/459 (99%)	406 (89%)	38 (8%)	12 (3%)	7	39
2	d	456/459 (99%)	411 (90%)	39 (9%)	6 (1%)	15	56
3	G	282/286 (99%)	265 (94%)	17 (6%)	0	100	100
3	O	282/286 (99%)	266 (94%)	15 (5%)	1 (0%)	39	78
3	W	282/286 (99%)	264 (94%)	16 (6%)	2 (1%)	26	70
3	e	282/286 (99%)	265 (94%)	15 (5%)	2 (1%)	26	70
4	H	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	13	53
4	P	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	13	53
4	X	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	13	53
4	f	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	13	53
All	All	12964/13360 (97%)	11533 (89%)	1237 (10%)	194 (2%)	13	53

5 of 194 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	455	TYR

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Mol	Chain	Res	Type
1	B	491	GLY
1	C	137	ILE
2	E	333	ALA
2	E	348	VAL

### 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	380/407 (93%)	319 (84%)	61 (16%)	3	14
1	B	371/407 (91%)	300 (81%)	71 (19%)	2	9
1	C	375/407 (92%)	307 (82%)	68 (18%)	2	11
1	I	380/407 (93%)	319 (84%)	61 (16%)	3	14
1	J	371/407 (91%)	300 (81%)	71 (19%)	2	9
1	K	375/407 (92%)	311 (83%)	64 (17%)	2	13
1	Q	380/407 (93%)	321 (84%)	59 (16%)	3	16
1	R	371/407 (91%)	299 (81%)	72 (19%)	2	9
1	S	375/407 (92%)	309 (82%)	66 (18%)	2	11
1	Y	380/407 (93%)	322 (85%)	58 (15%)	3	17
1	Z	371/407 (91%)	299 (81%)	72 (19%)	2	9
1	a	375/407 (92%)	310 (83%)	65 (17%)	2	12
2	D	380/380 (100%)	324 (85%)	56 (15%)	4	18
2	E	380/380 (100%)	306 (80%)	74 (20%)	2	8
2	F	380/380 (100%)	314 (83%)	66 (17%)	2	12
2	L	380/380 (100%)	324 (85%)	56 (15%)	4	18
2	M	380/380 (100%)	310 (82%)	70 (18%)	2	10
2	N	380/380 (100%)	311 (82%)	69 (18%)	2	10
2	T	380/380 (100%)	327 (86%)	53 (14%)	4	21
2	U	380/380 (100%)	308 (81%)	72 (19%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	V	380/380 (100%)	313 (82%)	67 (18%)	2	11
2	b	380/380 (100%)	325 (86%)	55 (14%)	4	19
2	c	380/380 (100%)	309 (81%)	71 (19%)	2	10
2	d	380/380 (100%)	315 (83%)	65 (17%)	2	13
3	G	236/239 (99%)	202 (86%)	34 (14%)	4	19
3	O	236/239 (99%)	202 (86%)	34 (14%)	4	19
3	W	236/239 (99%)	199 (84%)	37 (16%)	3	15
3	e	236/239 (99%)	200 (85%)	36 (15%)	3	17
4	H	109/109 (100%)	98 (90%)	11 (10%)	9	36
4	P	109/109 (100%)	98 (90%)	11 (10%)	9	36
4	X	109/109 (100%)	99 (91%)	10 (9%)	11	40
4	f	109/109 (100%)	98 (90%)	11 (10%)	9	36
All	All	10444/10836 (96%)	8698 (83%)	1746 (17%)	3	13

5 of 1746 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	N	162	LEU
1	R	384	LYS
2	c	344	LEU
2	N	324	GLN
1	Q	107	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 326 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	437	HIS
1	R	444	GLN
2	d	32	GLN
3	O	157	GLN
1	Q	344	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 49 ligands modelled in this entry, 16 are monoatomic - leaving 33 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	ANP	A	600	6	27,33,33	3.50	9 (33%)	30,52,52	3.33	9 (30%)
5	ANP	B	600	6	27,33,33	3.05	9 (33%)	30,52,52	3.25	10 (33%)
5	ANP	C	600	6	27,33,33	3.50	9 (33%)	30,52,52	3.33	9 (30%)
7	ADP	D	600	6	22,29,29	1.78	6 (27%)	27,45,45	2.57	8 (29%)
8	SO4	D	630	6	4,4,4	0.30	0	6,6,6	0.08	0
8	SO4	E	530	-	4,4,4	0.22	0	6,6,6	0.10	0
8	SO4	F	530	-	4,4,4	0.28	0	6,6,6	0.13	0
8	SO4	G	300	-	4,4,4	1.12	0	6,6,6	0.48	0
8	SO4	H	200	-	4,4,4	0.97	0	6,6,6	0.23	0
5	ANP	I	600	6	27,33,33	3.50	9 (33%)	30,52,52	3.33	9 (30%)
5	ANP	J	600	6	27,33,33	3.00	9 (33%)	30,52,52	3.27	10 (33%)
5	ANP	K	600	6	27,33,33	3.50	10 (37%)	30,52,52	3.37	10 (33%)
7	ADP	L	600	6	22,29,29	1.79	6 (27%)	27,45,45	2.58	8 (29%)
8	SO4	L	630	6	4,4,4	0.30	0	6,6,6	0.08	0
8	SO4	M	530	-	4,4,4	0.22	0	6,6,6	0.10	0
8	SO4	N	530	-	4,4,4	0.33	0	6,6,6	0.10	0
8	SO4	O	300	-	4,4,4	1.05	0	6,6,6	0.59	0
8	SO4	P	200	-	4,4,4	0.89	0	6,6,6	0.67	0
5	ANP	Q	600	6	27,33,33	3.50	9 (33%)	30,52,52	3.33	9 (30%)
5	ANP	R	600	6	27,33,33	3.03	8 (29%)	30,52,52	3.24	10 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	ANP	S	600	6	27,33,33	3.51	9 (33%)	30,52,52	3.33	8 (26%)
7	ADP	T	600	6	22,29,29	1.78	6 (27%)	27,45,45	2.54	8 (29%)
8	SO4	T	630	6	4,4,4	0.25	0	6,6,6	0.09	0
8	SO4	U	530	-	4,4,4	0.23	0	6,6,6	0.09	0
8	SO4	V	530	-	4,4,4	0.26	0	6,6,6	0.14	0
8	SO4	W	300	-	4,4,4	0.51	0	6,6,6	0.35	0
5	ANP	Y	600	6	27,33,33	3.51	9 (33%)	30,52,52	3.33	9 (30%)
5	ANP	Z	600	6	27,33,33	3.04	9 (33%)	30,52,52	3.28	10 (33%)
5	ANP	a	600	6	27,33,33	3.53	9 (33%)	30,52,52	3.30	8 (26%)
7	ADP	b	600	6	22,29,29	1.76	6 (27%)	27,45,45	2.57	8 (29%)
8	SO4	b	630	6	4,4,4	0.20	0	6,6,6	0.09	0
8	SO4	c	530	-	4,4,4	0.24	0	6,6,6	0.08	0
8	SO4	d	530	-	4,4,4	0.22	0	6,6,6	0.13	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
5	ANP	A	600	6	-	1/12/38/38	0/3/3/3
5	ANP	B	600	6	-	1/12/38/38	0/3/3/3
5	ANP	C	600	6	-	1/12/38/38	0/3/3/3
7	ADP	D	600	6	-	0/12/32/32	0/3/3/3
8	SO4	D	630	6	-	0/0/0/0	0/0/0/0
8	SO4	E	530	-	-	0/0/0/0	0/0/0/0
8	SO4	F	530	-	-	0/0/0/0	0/0/0/0
8	SO4	G	300	-	-	0/0/0/0	0/0/0/0
8	SO4	H	200	-	-	0/0/0/0	0/0/0/0
5	ANP	I	600	6	-	1/12/38/38	0/3/3/3
5	ANP	J	600	6	-	1/12/38/38	0/3/3/3
5	ANP	K	600	6	-	1/12/38/38	0/3/3/3
7	ADP	L	600	6	-	0/12/32/32	0/3/3/3
8	SO4	L	630	6	-	0/0/0/0	0/0/0/0
8	SO4	M	530	-	-	0/0/0/0	0/0/0/0
8	SO4	N	530	-	-	0/0/0/0	0/0/0/0
8	SO4	O	300	-	-	0/0/0/0	0/0/0/0
8	SO4	P	200	-	-	0/0/0/0	0/0/0/0
5	ANP	Q	600	6	-	1/12/38/38	0/3/3/3
5	ANP	R	600	6	-	1/12/38/38	0/3/3/3
5	ANP	S	600	6	-	1/12/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ADP	T	600	6	-	0/12/32/32	0/3/3/3
8	SO4	T	630	6	-	0/0/0/0	0/0/0/0
8	SO4	U	530	-	-	0/0/0/0	0/0/0/0
8	SO4	V	530	-	-	0/0/0/0	0/0/0/0
8	SO4	W	300	-	-	0/0/0/0	0/0/0/0
5	ANP	Y	600	6	-	1/12/38/38	0/3/3/3
5	ANP	Z	600	6	-	1/12/38/38	0/3/3/3
5	ANP	a	600	6	-	1/12/38/38	0/3/3/3
7	ADP	b	600	6	-	0/12/32/32	0/3/3/3
8	SO4	b	630	6	-	0/0/0/0	0/0/0/0
8	SO4	c	530	-	-	0/0/0/0	0/0/0/0
8	SO4	d	530	-	-	0/0/0/0	0/0/0/0

The worst 5 of 132 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	600	ANP	O2'-C2'	-5.05	1.30	1.43
5	K	600	ANP	O2'-C2'	-5.05	1.30	1.43
5	Y	600	ANP	O2'-C2'	-5.05	1.30	1.43
5	A	600	ANP	O2'-C2'	-5.02	1.30	1.43
5	I	600	ANP	O2'-C2'	-5.01	1.31	1.43

The worst 5 of 143 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	600	ANP	O1B-PB-N3B	-11.11	94.85	111.90
5	C	600	ANP	O1B-PB-N3B	-11.01	95.02	111.90
5	I	600	ANP	O1B-PB-N3B	-11.00	95.03	111.90
5	A	600	ANP	O1B-PB-N3B	-10.99	95.05	111.90
5	Q	600	ANP	O1B-PB-N3B	-10.98	95.05	111.90

There are no chirality outliers.

5 of 12 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	R	600	ANP	O1B-PB-N3B-PG
5	Z	600	ANP	O1B-PB-N3B-PG
5	B	600	ANP	O1B-PB-N3B-PG
5	J	600	ANP	O1B-PB-N3B-PG
5	K	600	ANP	O1B-PB-N3B-PG

There are no ring outliers.

19 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	600	ANP	4	0
5	B	600	ANP	3	0
5	C	600	ANP	3	0
7	D	600	ADP	5	0
8	D	630	SO4	1	0
8	F	530	SO4	1	0
5	I	600	ANP	4	0
5	J	600	ANP	3	0
5	K	600	ANP	2	0
7	L	600	ADP	5	0
8	L	630	SO4	1	0
8	N	530	SO4	1	0
5	Q	600	ANP	2	0
5	R	600	ANP	3	0
5	S	600	ANP	2	0
7	T	600	ADP	4	0
8	W	300	SO4	1	0
5	Y	600	ANP	3	0
5	Z	600	ANP	3	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	488/513 (95%)	-0.34	0 100 100	49, 93, 144, 177	0
1	B	486/513 (94%)	-0.21	9 (1%) 70 60	55, 116, 181, 216	0
1	C	487/513 (94%)	-0.30	6 (1%) 81 72	51, 102, 151, 231	0
1	I	488/513 (95%)	-0.13	11 (2%) 64 54	66, 120, 167, 205	0
1	J	486/513 (94%)	-0.15	15 (3%) 52 43	47, 103, 183, 223	0
1	K	487/513 (94%)	-0.31	10 (2%) 67 57	46, 91, 149, 211	0
1	Q	488/513 (95%)	-0.29	10 (2%) 68 58	50, 104, 153, 214	0
1	R	486/513 (94%)	0.11	22 (4%) 37 28	66, 123, 195, 227	0
1	S	487/513 (94%)	-0.04	12 (2%) 61 51	78, 131, 180, 226	0
1	Y	488/513 (95%)	0.13	25 (5%) 32 23	79, 142, 184, 224	0
1	Z	486/513 (94%)	0.59	61 (12%) 5 3	77, 152, 215, 254	0
1	a	487/513 (94%)	0.30	33 (6%) 20 15	89, 146, 200, 249	0
2	D	458/459 (99%)	-0.44	3 (0%) 89 84	44, 92, 142, 186	0
2	E	458/459 (99%)	-0.37	3 (0%) 89 84	53, 102, 152, 184	0
2	F	458/459 (99%)	-0.42	5 (1%) 82 75	41, 103, 158, 216	0
2	L	458/459 (99%)	-0.19	12 (2%) 59 50	46, 111, 167, 217	0
2	M	458/459 (99%)	-0.21	7 (1%) 76 67	55, 114, 161, 219	0
2	N	458/459 (99%)	-0.44	6 (1%) 79 71	33, 73, 131, 186	0
2	T	458/459 (99%)	-0.12	12 (2%) 59 50	73, 124, 181, 229	0
2	U	458/459 (99%)	-0.21	5 (1%) 82 75	54, 102, 170, 232	0
2	V	458/459 (99%)	-0.01	17 (3%) 45 35	67, 124, 180, 233	0
2	b	458/459 (99%)	0.47	47 (10%) 9 6	102, 158, 204, 240	0
2	c	458/459 (99%)	-0.00	17 (3%) 45 35	68, 119, 174, 213	0
2	d	458/459 (99%)	0.32	33 (7%) 18 13	92, 151, 200, 243	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
3	G	284/286 (99%)	-0.54	4 (1%) 78 69	29, 54, 137, 200	0
3	O	284/286 (99%)	-0.46	7 (2%) 61 51	26, 57, 140, 209	0
3	W	284/286 (99%)	0.03	17 (5%) 25 18	51, 116, 192, 232	0
3	e	284/286 (99%)	0.28	25 (8%) 12 8	84, 142, 205, 230	0
4	H	138/138 (100%)	-0.41	1 (0%) 89 84	35, 72, 120, 144	0
4	P	138/138 (100%)	-0.37	1 (0%) 89 84	43, 71, 129, 156	0
4	X	138/138 (100%)	0.23	10 (7%) 18 13	77, 136, 175, 227	0
4	f	138/138 (100%)	0.52	20 (14%) 3 2	94, 151, 198, 217	0
All	All	13028/13360 (97%)	-0.10	466 (3%) 46 37	26, 116, 183, 254	0

The worst 5 of 466 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	a	312	PHE	7.3
1	C	312	PHE	6.8
2	b	48	GLY	6.6
1	K	313	THR	6.6
1	R	410	ALA	5.9

## 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
8	SO4	P	200	5/5	0.92	0.35	5.96	120,120,123,124	0
8	SO4	H	200	5/5	0.96	0.24	5.27	114,115,117,119	0
8	SO4	W	300	5/5	0.80	0.37	4.12	207,210,212,214	0
8	SO4	G	300	5/5	0.90	0.26	3.94	95,101,102,103	0
8	SO4	O	300	5/5	0.93	0.26	3.93	109,115,118,119	0
8	SO4	c	530	5/5	0.83	0.29	0.60	113,113,115,116	0
8	SO4	E	530	5/5	0.94	0.27	0.55	109,109,109,110	0
8	SO4	U	530	5/5	0.94	0.23	0.27	106,106,107,107	0
8	SO4	M	530	5/5	0.85	0.28	0.07	117,118,119,119	0
5	ANP	Z	600	31/31	0.88	0.24	-0.21	147,151,153,154	0
5	ANP	R	600	31/31	0.92	0.20	-0.26	91,101,110,112	0
5	ANP	A	600	31/31	0.88	0.21	-0.29	87,93,109,129	0
5	ANP	C	600	31/31	0.94	0.16	-0.44	87,93,109,129	0
5	ANP	Y	600	31/31	0.90	0.24	-0.45	87,93,109,129	0
5	ANP	K	600	31/31	0.96	0.15	-0.54	63,81,109,131	0
5	ANP	Q	600	31/31	0.91	0.19	-0.58	87,93,109,129	0
5	ANP	I	600	31/31	0.92	0.17	-0.65	87,93,109,129	0
5	ANP	S	600	31/31	0.92	0.18	-0.65	109,114,121,135	0
5	ANP	J	600	31/31	0.95	0.16	-0.71	83,96,100,103	0
5	ANP	B	600	31/31	0.94	0.16	-0.78	96,107,111,112	0
7	ADP	b	600	27/27	0.91	0.18	-0.80	136,139,142,143	0
5	ANP	a	600	31/31	0.91	0.20	-0.81	123,126,130,136	0
6	MG	b	601	1/1	0.95	0.20	-0.82	127,127,127,127	0
7	ADP	L	600	27/27	0.95	0.13	-0.94	77,86,95,98	0
8	SO4	F	530	5/5	0.98	0.10	-0.99	79,81,82,82	0
8	SO4	d	530	5/5	0.97	0.18	-1.00	107,108,108,109	0
8	SO4	V	530	5/5	0.98	0.08	-1.01	82,83,85,87	0
7	ADP	D	600	27/27	0.96	0.12	-1.05	75,81,87,90	0
8	SO4	N	530	5/5	0.97	0.09	-1.06	64,64,67,67	0
6	MG	Y	601	1/1	0.93	0.17	-1.19	64,64,64,64	0
7	ADP	T	600	27/27	0.95	0.12	-1.33	114,118,121,123	0
6	MG	T	601	1/1	0.86	0.14	-1.36	80,80,80,80	0
8	SO4	T	630	5/5	0.97	0.09	-1.58	85,88,88,89	0
8	SO4	b	630	5/5	0.93	0.12	-1.99	98,99,100,101	0
8	SO4	D	630	5/5	0.98	0.10	-2.71	72,74,75,77	0
8	SO4	L	630	5/5	0.99	0.07	-2.71	81,83,84,85	0
6	MG	D	601	1/1	0.98	0.12	-2.85	51,51,51,51	0
6	MG	L	601	1/1	0.96	0.07	-3.55	66,66,66,66	0
6	MG	I	601	1/1	0.91	0.16	-	64,64,64,64	0
6	MG	S	601	1/1	0.94	0.12	-	60,60,60,60	0
6	MG	a	601	1/1	0.83	0.18	-	83,83,83,83	0
6	MG	R	601	1/1	0.94	0.09	-	118,118,118,118	0
6	MG	A	601	1/1	0.89	0.22	-	64,64,64,64	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MG	Q	601	1/1	0.83	0.26	-	64,64,64,64	0
6	MG	B	601	1/1	0.93	0.16	-	125,125,125,125	0
6	MG	K	601	1/1	0.94	0.09	-	44,44,44,44	0
6	MG	C	601	1/1	0.95	0.10	-	64,64,64,64	0
6	MG	Z	601	1/1	0.90	0.09	-	147,147,147,147	0
6	MG	J	601	1/1	0.95	0.14	-	122,122,122,122	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.