



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 11:22 AM GMT

PDB ID : 3OEH  
Title : Structure of four mutant forms of yeast F1 ATPase: beta-V279F  
Authors : Arsenieva, D.; Symersky, J.; Wang, Y.; Pagadala, V.; Mueller, D.M.  
Deposited on : 2010-08-12  
Resolution : 3.00 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

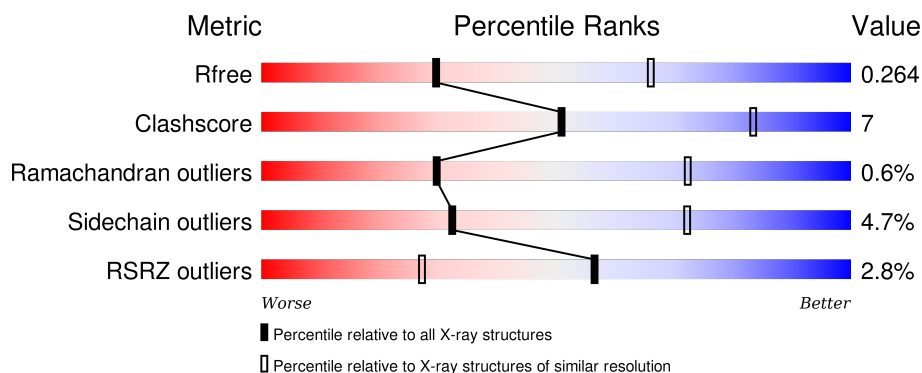
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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.






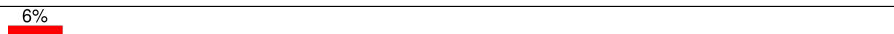
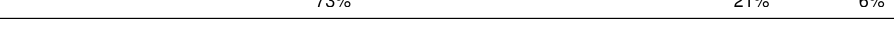
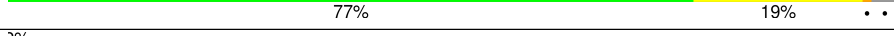



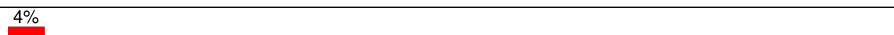
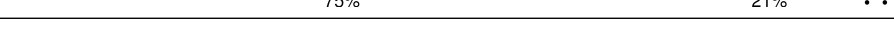




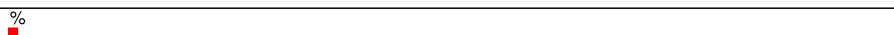






Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	510	<div> <div>78%</div> <div>15%</div> <div>• 5%</div> </div>
1	B	510	<div> <div>3%</div> <div>75%</div> <div>18%</div> <div>• 5%</div> </div>
1	C	510	<div> <div>80%</div> <div>14%</div> <div>• 5%</div> </div>
1	J	510	<div> <div>79%</div> <div>15%</div> <div>6%</div> </div>
1	K	510	<div> <div>3%</div> <div>74%</div> <div>21%</div> <div>• 5%</div> </div>

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Mol	Chain	Length	Quality of chain
1	L	510	
1	S	510	
1	T	510	
1	U	510	
2	D	484	
2	E	484	
2	F	484	
2	M	484	
2	N	484	
2	O	484	
2	V	484	
2	W	484	
2	X	484	
3	G	278	
3	P	278	
3	Y	278	
4	H	138	
4	Q	138	
4	Z	138	
5	1	61	
5	I	61	
5	R	61	

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
7	MG	D	700	-	-	-	X
7	MG	F	700	-	-	-	X
7	MG	M	700	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 72707 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	482	Total	C	N	O	S	0	0	0
			3664	2314	648	699	3			
1	B	483	Total	C	N	O	S	0	0	0
			3669	2317	649	700	3			
1	C	484	Total	C	N	O	S	0	0	0
			3680	2325	650	702	3			
1	J	481	Total	C	N	O	S	0	0	0
			3655	2309	646	697	3			
1	K	486	Total	C	N	O	S	0	0	0
			3688	2327	652	706	3			
1	L	482	Total	C	N	O	S	0	0	0
			3664	2314	648	699	3			
1	S	478	Total	C	N	O	S	0	0	0
			3635	2297	643	692	3			
1	T	479	Total	C	N	O	S	0	0	0
			3642	2302	644	693	3			
1	U	481	Total	C	N	O	S	0	0	0
			3655	2308	646	698	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	470	Total	C	N	O	S	0	0	0
			3549	2252	603	688	6			
2	E	468	Total	C	N	O	S	0	0	0
			3508	2227	598	677	6			
2	F	469	Total	C	N	O	S	0	0	0
			3531	2242	602	681	6			
2	M	470	Total	C	N	O	S	0	0	0
			3543	2249	600	688	6			
2	N	470	Total	C	N	O	S	0	0	0
			3545	2249	602	688	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	468	Total	C	N	O	S	0	0	0
			3538	2246	602	684	6			
2	V	470	Total	C	N	O	S	0	0	0
			3550	2251	604	689	6			
2	W	467	Total	C	N	O	S	0	0	0
			3535	2244	601	684	6			
2	X	469	Total	C	N	O	S	0	0	0
			3547	2251	603	687	6			

There are 81 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-5	ALA	-	EXPRESSION TAG	UNP P00830
D	-4	SER	-	EXPRESSION TAG	UNP P00830
D	-3	HIS	-	EXPRESSION TAG	UNP P00830
D	-2	HIS	-	EXPRESSION TAG	UNP P00830
D	-1	HIS	-	EXPRESSION TAG	UNP P00830
D	0	HIS	-	EXPRESSION TAG	UNP P00830
D	1	HIS	-	EXPRESSION TAG	UNP P00830
D	2	HIS	-	EXPRESSION TAG	UNP P00830
D	279	PHE	VAL	ENGINEERED MUTATION	UNP P00830
E	-5	ALA	-	EXPRESSION TAG	UNP P00830
E	-4	SER	-	EXPRESSION TAG	UNP P00830
E	-3	HIS	-	EXPRESSION TAG	UNP P00830
E	-2	HIS	-	EXPRESSION TAG	UNP P00830
E	-1	HIS	-	EXPRESSION TAG	UNP P00830
E	0	HIS	-	EXPRESSION TAG	UNP P00830
E	1	HIS	-	EXPRESSION TAG	UNP P00830
E	2	HIS	-	EXPRESSION TAG	UNP P00830
E	279	PHE	VAL	ENGINEERED MUTATION	UNP P00830
F	-5	ALA	-	EXPRESSION TAG	UNP P00830
F	-4	SER	-	EXPRESSION TAG	UNP P00830
F	-3	HIS	-	EXPRESSION TAG	UNP P00830
F	-2	HIS	-	EXPRESSION TAG	UNP P00830
F	-1	HIS	-	EXPRESSION TAG	UNP P00830
F	0	HIS	-	EXPRESSION TAG	UNP P00830
F	1	HIS	-	EXPRESSION TAG	UNP P00830
F	2	HIS	-	EXPRESSION TAG	UNP P00830
F	279	PHE	VAL	ENGINEERED MUTATION	UNP P00830
M	-5	ALA	-	EXPRESSION TAG	UNP P00830
M	-4	SER	-	EXPRESSION TAG	UNP P00830
M	-3	HIS	-	EXPRESSION TAG	UNP P00830
M	-2	HIS	-	EXPRESSION TAG	UNP P00830

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Chain	Residue	Modelled	Actual	Comment	Reference
M	-1	HIS	-	EXPRESSION TAG	UNP P00830
M	0	HIS	-	EXPRESSION TAG	UNP P00830
M	1	HIS	-	EXPRESSION TAG	UNP P00830
M	2	HIS	-	EXPRESSION TAG	UNP P00830
M	279	PHE	VAL	ENGINEERED MUTATION	UNP P00830
N	-5	ALA	-	EXPRESSION TAG	UNP P00830
N	-4	SER	-	EXPRESSION TAG	UNP P00830
N	-3	HIS	-	EXPRESSION TAG	UNP P00830
N	-2	HIS	-	EXPRESSION TAG	UNP P00830
N	-1	HIS	-	EXPRESSION TAG	UNP P00830
N	0	HIS	-	EXPRESSION TAG	UNP P00830
N	1	HIS	-	EXPRESSION TAG	UNP P00830
N	2	HIS	-	EXPRESSION TAG	UNP P00830
N	279	PHE	VAL	ENGINEERED MUTATION	UNP P00830
O	-5	ALA	-	EXPRESSION TAG	UNP P00830
O	-4	SER	-	EXPRESSION TAG	UNP P00830
O	-3	HIS	-	EXPRESSION TAG	UNP P00830
O	-2	HIS	-	EXPRESSION TAG	UNP P00830
O	-1	HIS	-	EXPRESSION TAG	UNP P00830
O	0	HIS	-	EXPRESSION TAG	UNP P00830
O	1	HIS	-	EXPRESSION TAG	UNP P00830
O	2	HIS	-	EXPRESSION TAG	UNP P00830
O	279	PHE	VAL	ENGINEERED MUTATION	UNP P00830
V	-5	ALA	-	EXPRESSION TAG	UNP P00830
V	-4	SER	-	EXPRESSION TAG	UNP P00830
V	-3	HIS	-	EXPRESSION TAG	UNP P00830
V	-2	HIS	-	EXPRESSION TAG	UNP P00830
V	-1	HIS	-	EXPRESSION TAG	UNP P00830
V	0	HIS	-	EXPRESSION TAG	UNP P00830
V	1	HIS	-	EXPRESSION TAG	UNP P00830
V	2	HIS	-	EXPRESSION TAG	UNP P00830
V	279	PHE	VAL	ENGINEERED MUTATION	UNP P00830
W	-5	ALA	-	EXPRESSION TAG	UNP P00830
W	-4	SER	-	EXPRESSION TAG	UNP P00830
W	-3	HIS	-	EXPRESSION TAG	UNP P00830
W	-2	HIS	-	EXPRESSION TAG	UNP P00830
W	-1	HIS	-	EXPRESSION TAG	UNP P00830
W	0	HIS	-	EXPRESSION TAG	UNP P00830
W	1	HIS	-	EXPRESSION TAG	UNP P00830
W	2	HIS	-	EXPRESSION TAG	UNP P00830
W	279	PHE	VAL	ENGINEERED MUTATION	UNP P00830
X	-5	ALA	-	EXPRESSION TAG	UNP P00830

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-4	SER	-	EXPRESSION TAG	UNP P00830
X	-3	HIS	-	EXPRESSION TAG	UNP P00830
X	-2	HIS	-	EXPRESSION TAG	UNP P00830
X	-1	HIS	-	EXPRESSION TAG	UNP P00830
X	0	HIS	-	EXPRESSION TAG	UNP P00830
X	1	HIS	-	EXPRESSION TAG	UNP P00830
X	2	HIS	-	EXPRESSION TAG	UNP P00830
X	279	PHE	VAL	ENGINEERED MUTATION	UNP P00830

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	266	Total	C	N	O	S	0	0	0
			2059	1293	359	397	10			
3	P	246	Total	C	N	O	S	0	0	0
			1872	1175	327	361	9			
3	Y	201	Total	C	N	O	S	0	0	0
			1523	947	274	293	9			

- Molecule 4 is a protein called ATP synthase subunit delta.

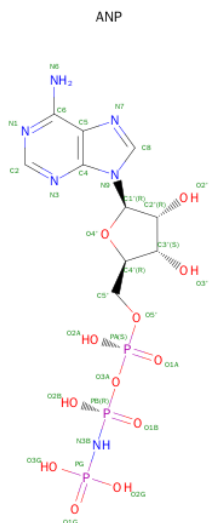
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	116	Total	C	N	O	S	0	0	0
			763	477	132	152	2			
4	Q	84	Total	C	N	O		0	0	0
			454	277	89	88				
4	Z	17	Total	C	N	O		0	0	0
			85	51	17	17				

- Molecule 5 is a protein called ATP synthase subunit epsilon.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	49	Total	C	N	O	0	0	0
			339	212	57	70			
5	R	34	Total	C	N	O	0	0	0
			189	116	34	39			
5	1	27	Total	C	N	O	0	0	0
			145	86	31	28			

- Molecule 6 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>).





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

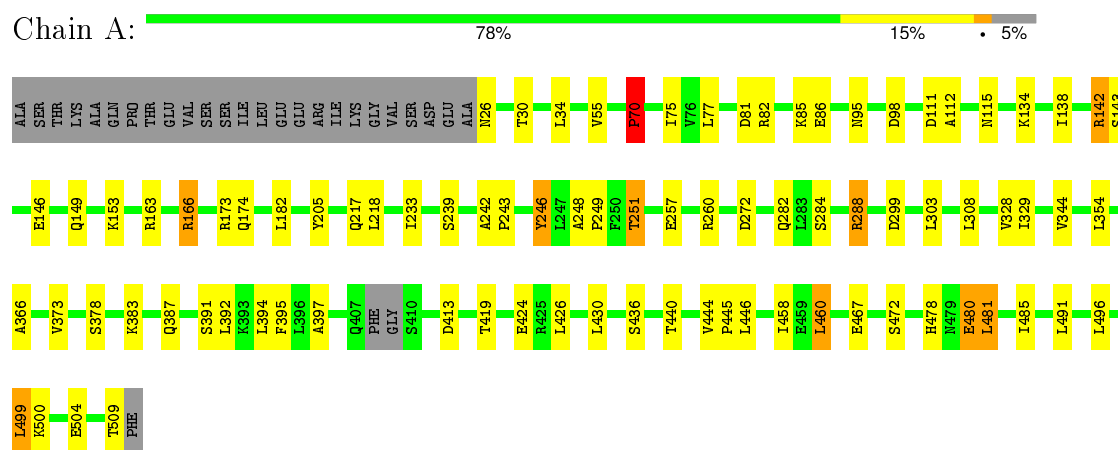
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		
7	K	1	Total	Mg	0	0
			1	1		
7	B	1	Total	Mg	0	0
			1	1		
7	C	1	Total	Mg	0	0
			1	1		
7	V	1	Total	Mg	0	0
			1	1		
7	A	1	Total	Mg	0	0
			1	1		
7	T	1	Total	Mg	0	0
			1	1		
7	U	1	Total	Mg	0	0
			1	1		
7	X	1	Total	Mg	0	0
			1	1		
7	O	1	Total	Mg	0	0
			1	1		
7	L	1	Total	Mg	0	0
			1	1		
7	S	1	Total	Mg	0	0
			1	1		
7	F	1	Total	Mg	0	0
			1	1		
7	M	1	Total	Mg	0	0
			1	1		

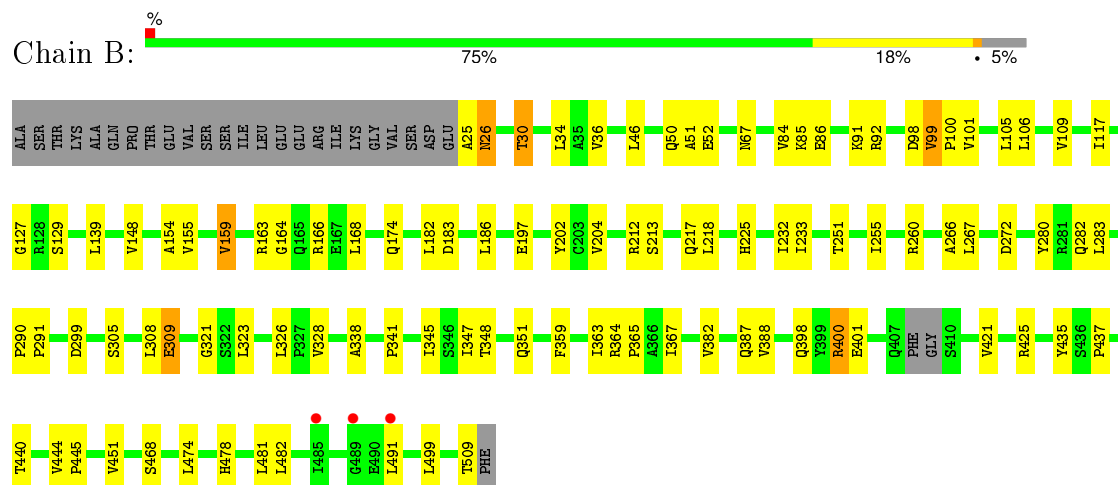
### 3 Residue-property plots

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

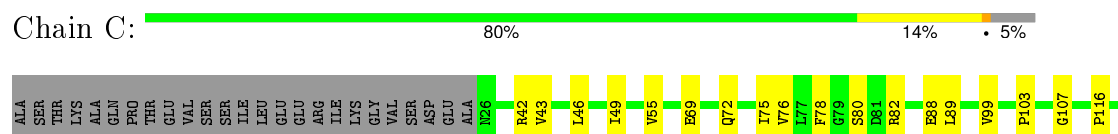
- Molecule 1: ATP synthase subunit alpha

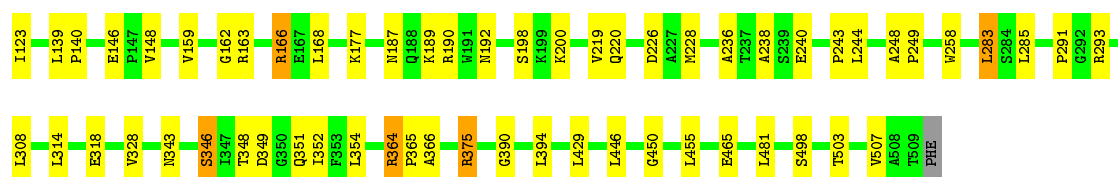


- Molecule 1: ATP synthase subunit alpha



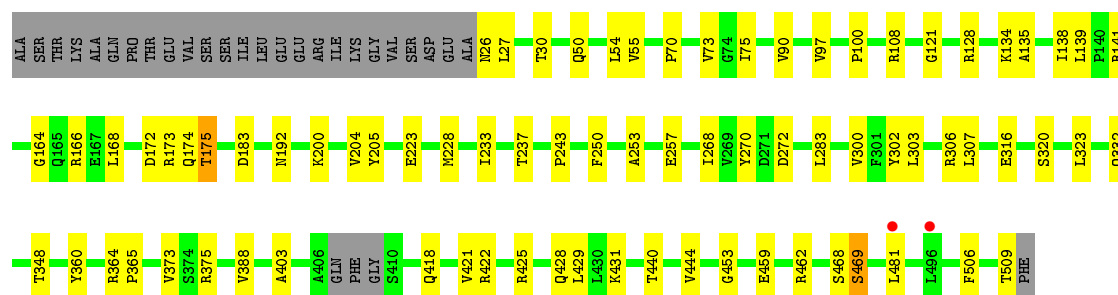
- Molecule 1: ATP synthase subunit alpha





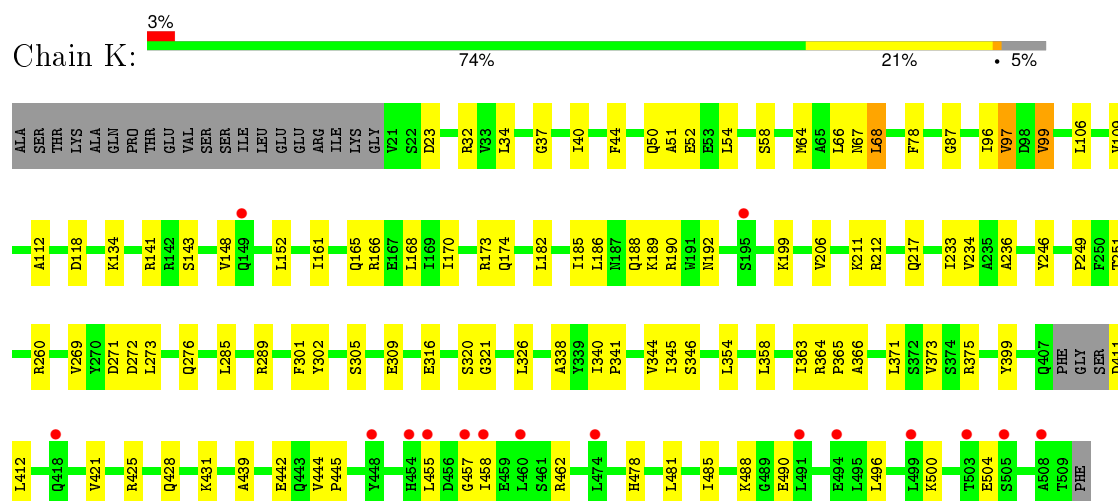
• Molecule 1: ATP synthase subunit alpha

Chain J:



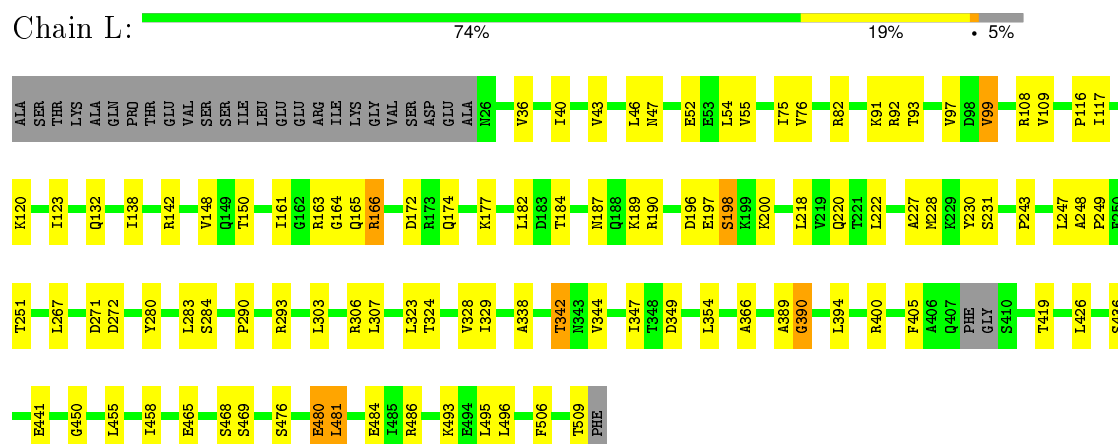
• Molecule 1: ATP synthase subunit alpha

Chain K:

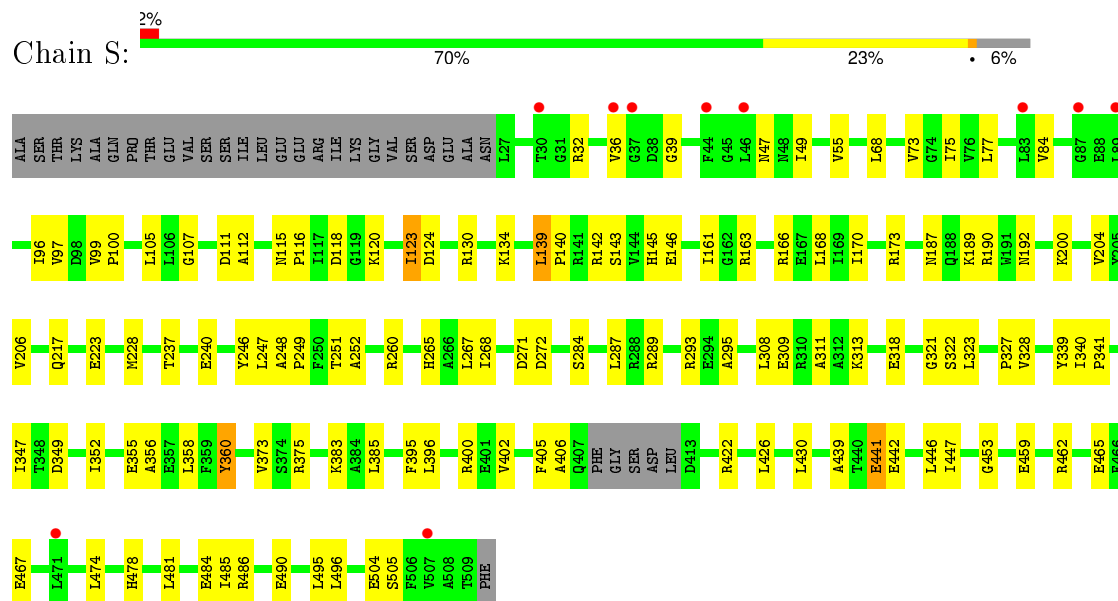


• Molecule 1: ATP synthase subunit alpha

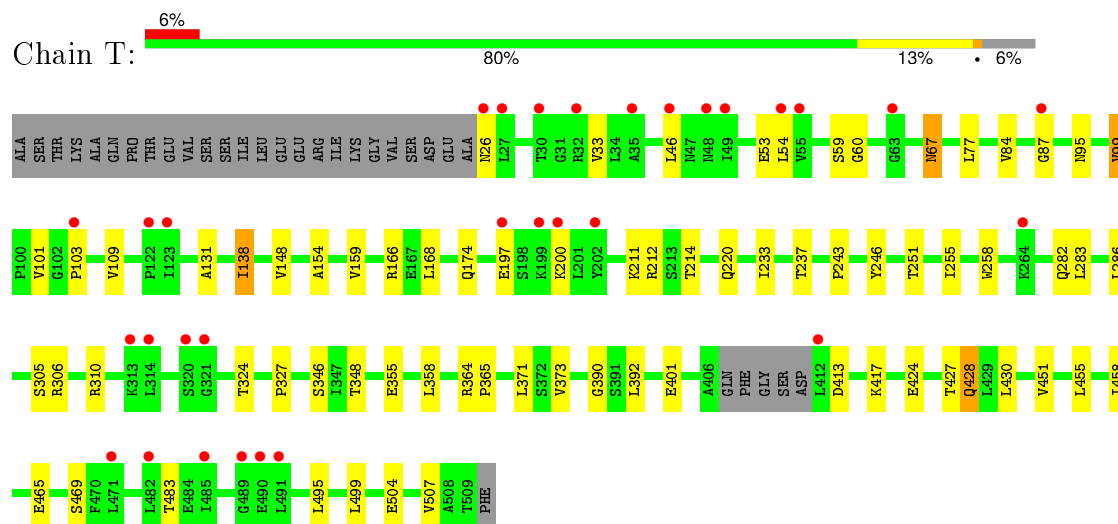
Chain L:



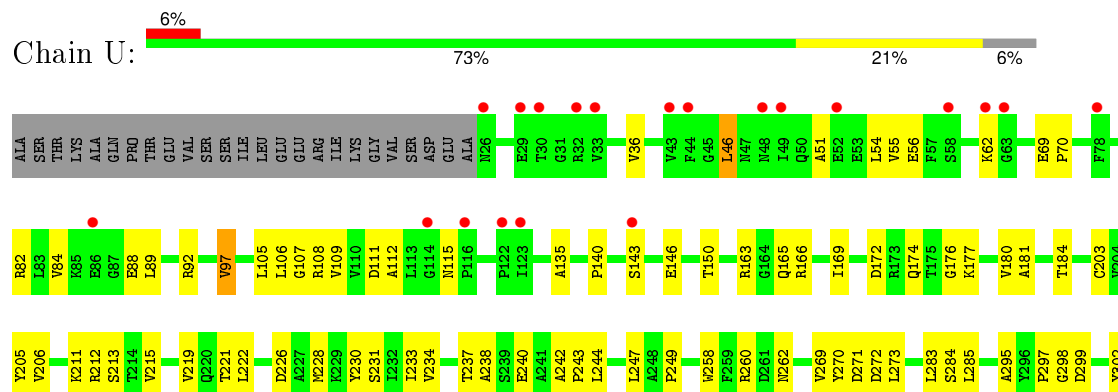
- Molecule 1: ATP synthase subunit alpha

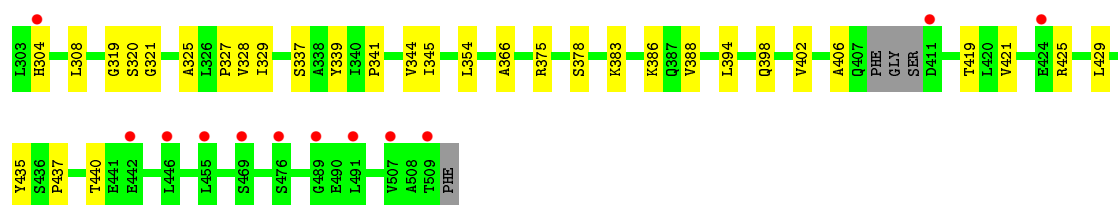


- Molecule 1: ATP synthase subunit alpha



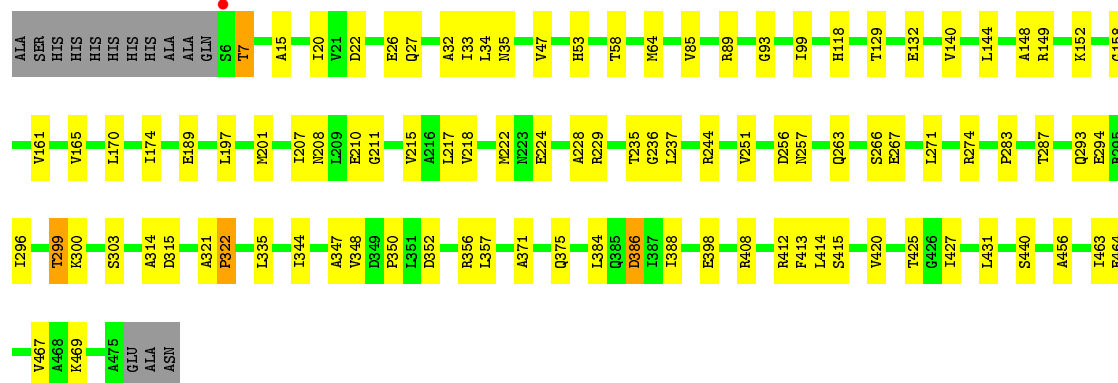
- Molecule 1: ATP synthase subunit alpha





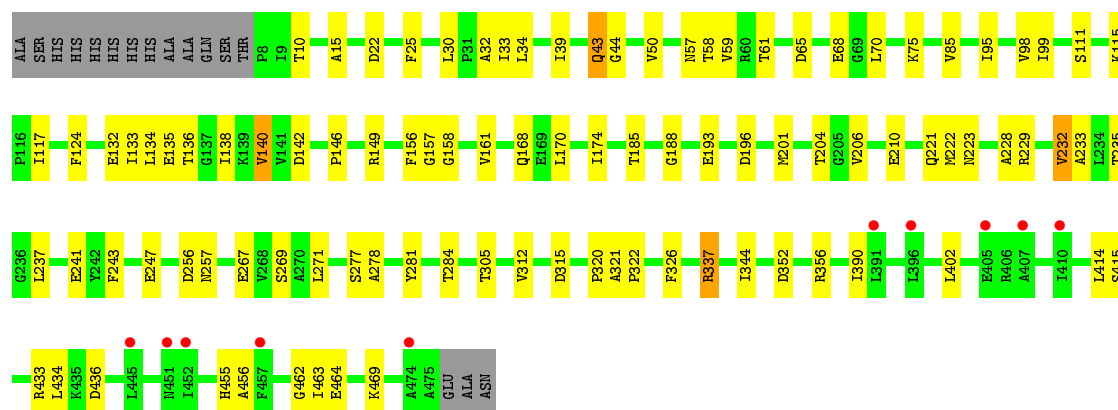
• Molecule 2: ATP synthase subunit beta

Chain D: 77% 19%



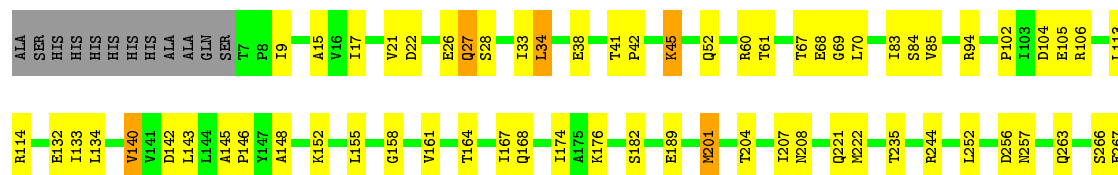
• Molecule 2: ATP synthase subunit beta

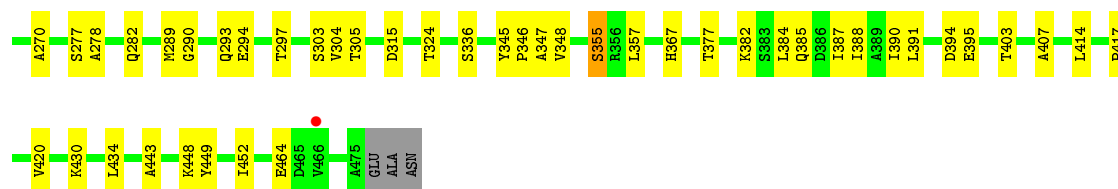
Chain E: 2% 76% 19%



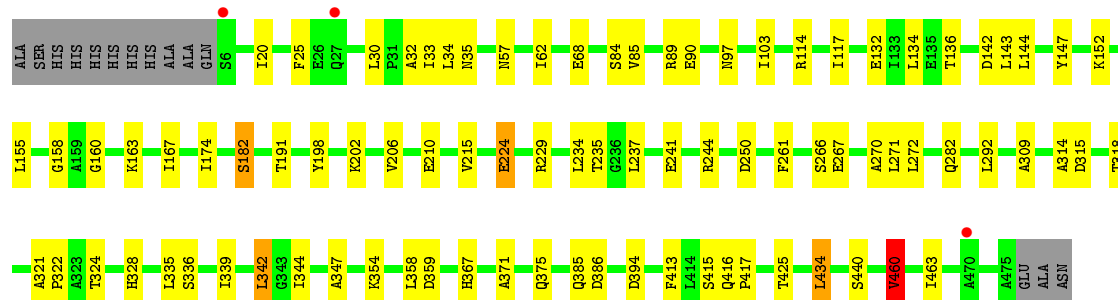
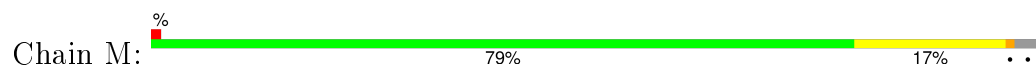
• Molecule 2: ATP synthase subunit beta

Chain F: 74% 21%

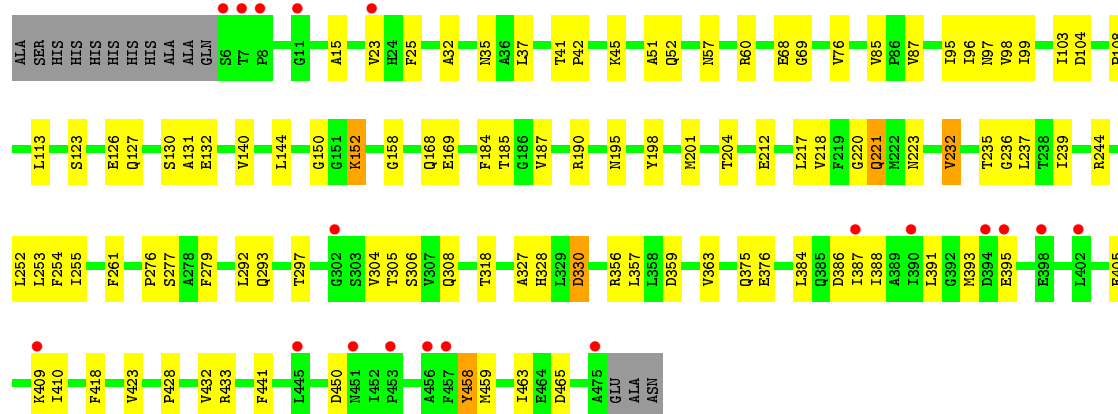
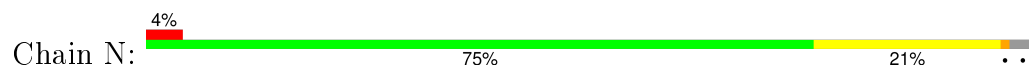




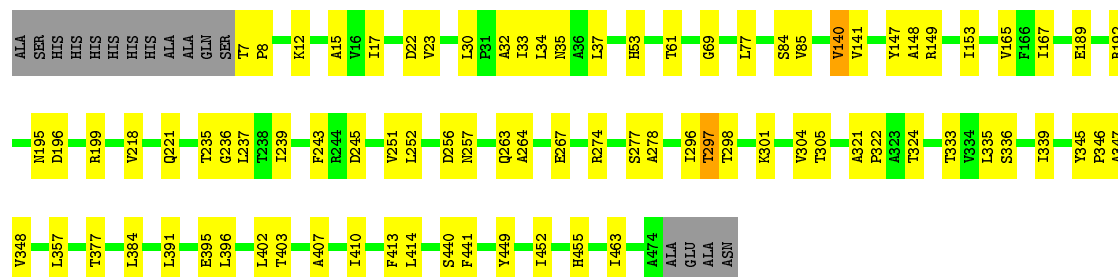
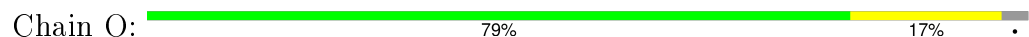
• Molecule 2: ATP synthase subunit beta



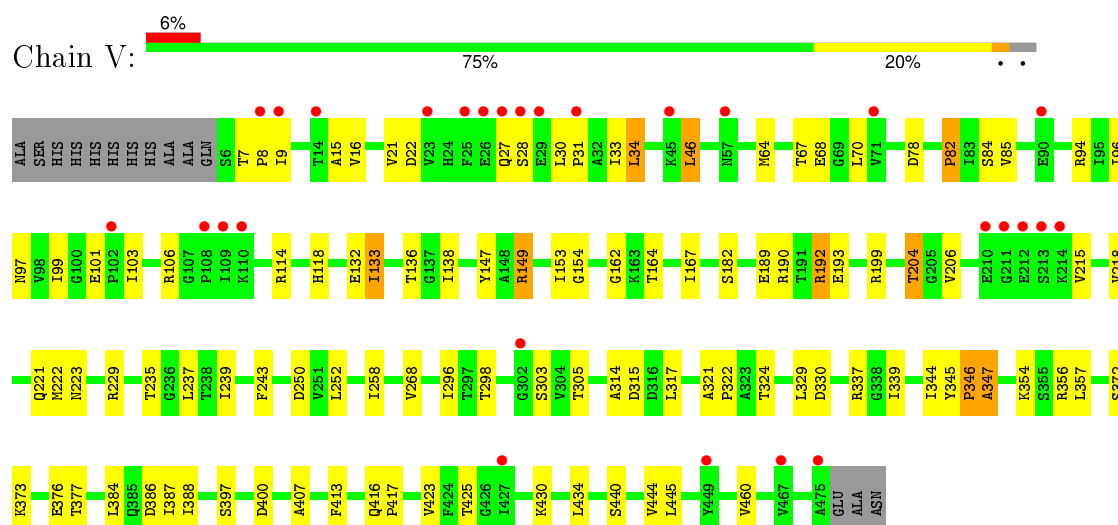
• Molecule 2: ATP synthase subunit beta



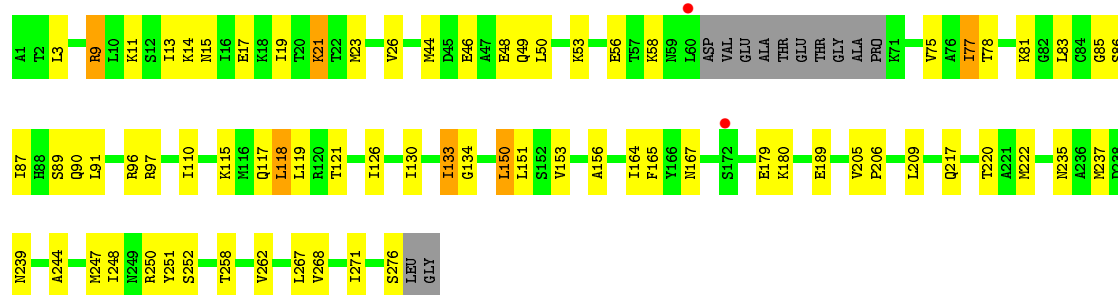
• Molecule 2: ATP synthase subunit beta



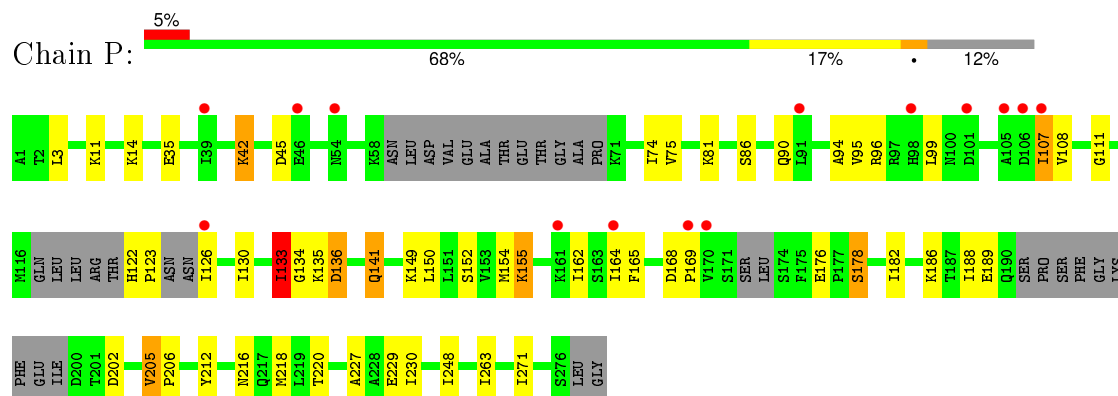
• Molecule 2: ATP synthase subunit beta



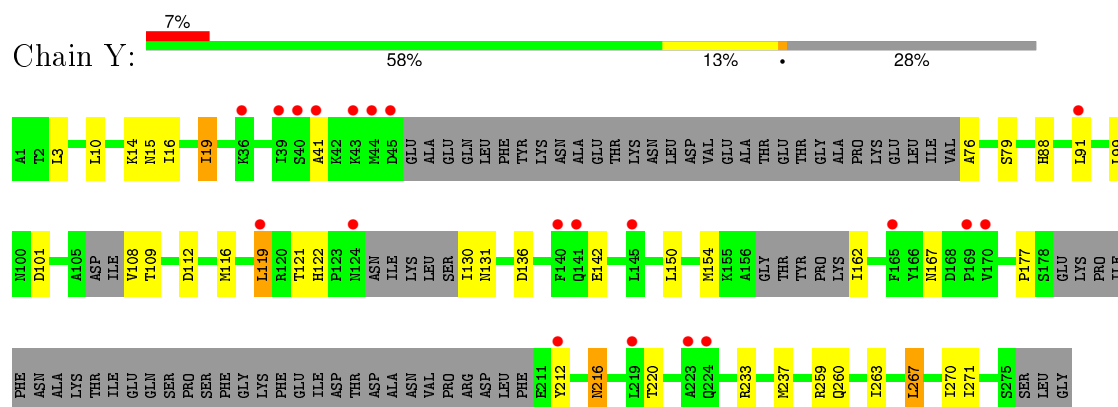




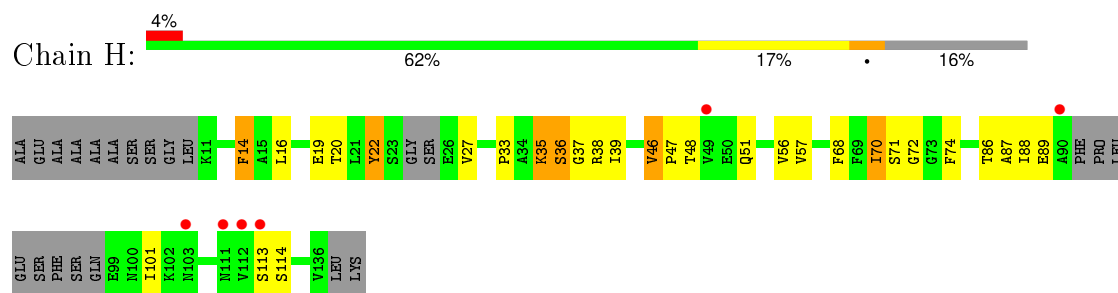
• Molecule 3: ATP synthase subunit gamma



• Molecule 3: ATP synthase subunit gamma

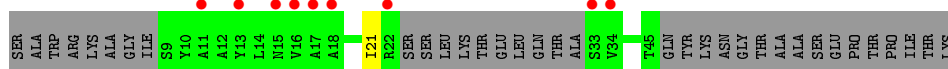


• Molecule 4: ATP synthase subunit delta



• Molecule 4: ATP synthase subunit delta





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	110.93Å 291.90Å 188.76Å 90.00° 101.91° 90.00°	Depositor
Resolution (Å)	20.00 – 3.00 49.39 – 3.00	Depositor EDS
% Data completeness (in resolution range)	88.8 (20.00-3.00) 88.6 (49.39-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.05	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.29 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.209 , 0.270 0.206 , 0.264	Depositor DCC
$R_{free}$ test set	4154 reflections (2.05%)	DCC
Wilson B-factor (Å <sup>2</sup> )	82.8	Xtriage
Anisotropy	0.128	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 55.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 207723 reflections	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	72707	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	110.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.33% 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 [i](#)

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

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

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	0.46	0/3718	0.65	0/5032
1	B	0.39	0/3723	0.59	0/5039
1	C	0.42	0/3736	0.62	1/5057 (0.0%)
1	J	0.36	0/3709	0.56	0/5020
1	K	0.35	0/3742	0.54	0/5065
1	L	0.43	0/3718	0.61	1/5032 (0.0%)
1	S	0.37	0/3689	0.54	0/4992
1	T	0.34	0/3696	0.50	0/5002
1	U	0.35	0/3709	0.54	0/5021
2	D	0.47	0/3606	0.61	0/4890
2	E	0.42	0/3565	0.58	0/4840
2	F	0.40	0/3588	0.58	0/4868
2	M	0.39	0/3600	0.58	0/4883
2	N	0.37	0/3602	0.53	1/4886 (0.0%)
2	O	0.37	0/3595	0.56	0/4875
2	V	0.37	0/3607	0.53	0/4891
2	W	0.36	0/3592	0.52	0/4869
2	X	0.36	0/3604	0.53	0/4887
3	G	0.39	0/2084	0.53	0/2803
3	P	0.36	0/1889	0.53	0/2537
3	Y	0.34	0/1533	0.51	0/2056
4	H	0.39	0/772	0.59	0/1058
4	Q	0.36	0/453	0.51	0/621
4	Z	0.35	0/84	0.45	0/116
5	1	0.30	0/143	0.42	0/195
5	I	0.42	0/343	0.59	0/470
5	R	0.39	0/189	0.50	0/261
All	All	0.39	0/73289	0.56	3/99266 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	283	LEU	CA-CB-CG	5.70	128.40	115.30
2	N	37	LEU	CA-CB-CG	5.34	127.57	115.30
1	C	283	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3664	0	3747	59	0
1	B	3669	0	3752	59	0
1	C	3680	0	3763	40	0
1	J	3655	0	3739	43	0
1	K	3688	0	3763	63	0
1	L	3664	0	3747	54	0
1	S	3635	0	3724	70	0
1	T	3642	0	3733	36	0
1	U	3655	0	3734	62	0
2	D	3549	0	3614	59	0
2	E	3508	0	3550	51	0
2	F	3531	0	3592	58	0
2	M	3543	0	3603	49	0
2	N	3545	0	3604	63	0
2	O	3538	0	3606	47	0
2	V	3550	0	3611	64	0
2	W	3535	0	3605	47	0
2	X	3547	0	3615	39	0
3	G	2059	0	2127	43	0
3	P	1872	0	1917	34	0
3	Y	1523	0	1569	16	0
4	H	763	0	653	21	0
4	Q	454	0	259	2	0
4	Z	85	0	45	0	0
5	1	145	0	87	0	0
5	I	339	0	280	8	0
5	R	189	0	114	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	31	0	13	1	0
6	B	31	0	13	4	0
6	C	31	0	13	0	0
6	D	31	0	13	0	0
6	F	31	0	13	1	0
6	J	31	0	13	1	0
6	K	31	0	13	3	0
6	L	31	0	13	1	0
6	M	31	0	13	4	0
6	O	31	0	13	3	0
6	S	31	0	13	0	0
6	T	31	0	13	1	0
6	U	31	0	13	1	0
6	V	31	0	13	1	0
6	X	31	0	13	4	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
7	J	1	0	0	0	0
7	K	1	0	0	0	0
7	L	1	0	0	0	0
7	M	1	0	0	0	0
7	O	1	0	0	0	0
7	S	1	0	0	0	0
7	T	1	0	0	0	0
7	U	1	0	0	0	0
7	V	1	0	0	0	0
7	X	1	0	0	0	0
All	All	72707	0	73348	1008	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 7.

The worst 5 of 1008 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)
2:M:85:VAL:HG11	2:M:235:THR:HG23	1.30	1.12
2:D:85:VAL:HG11	2:D:235:THR:HG23	1.15	1.09
1:A:395:PHE:HZ	1:A:419:THR:HA	1.15	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.38	1.01
1:B:174:GLN:HA	6:B:600:ANP:HNB1	1.28	0.97

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	478/510 (94%)	454 (95%)	23 (5%)	1 (0%)	52	88
1	B	479/510 (94%)	448 (94%)	30 (6%)	1 (0%)	52	88
1	C	482/510 (94%)	453 (94%)	28 (6%)	1 (0%)	52	88
1	J	477/510 (94%)	460 (96%)	16 (3%)	1 (0%)	52	88
1	K	482/510 (94%)	442 (92%)	35 (7%)	5 (1%)	19	61
1	L	478/510 (94%)	450 (94%)	27 (6%)	1 (0%)	52	88
1	S	474/510 (93%)	447 (94%)	25 (5%)	2 (0%)	39	80
1	T	475/510 (93%)	438 (92%)	33 (7%)	4 (1%)	24	66
1	U	477/510 (94%)	432 (91%)	39 (8%)	6 (1%)	15	53
2	D	468/484 (97%)	439 (94%)	28 (6%)	1 (0%)	52	88
2	E	466/484 (96%)	436 (94%)	28 (6%)	2 (0%)	39	80
2	F	467/484 (96%)	435 (93%)	27 (6%)	5 (1%)	17	58
2	M	468/484 (97%)	437 (93%)	30 (6%)	1 (0%)	52	88
2	N	468/484 (97%)	431 (92%)	33 (7%)	4 (1%)	21	64
2	O	466/484 (96%)	442 (95%)	24 (5%)	0	100	100
2	V	468/484 (97%)	423 (90%)	38 (8%)	7 (2%)	13	50
2	W	465/484 (96%)	432 (93%)	30 (6%)	3 (1%)	30	72
2	X	467/484 (96%)	432 (92%)	33 (7%)	2 (0%)	39	80

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	262/278 (94%)	245 (94%)	17 (6%)	0	100	100
3	P	234/278 (84%)	210 (90%)	19 (8%)	5 (2%)	9	40
3	Y	189/278 (68%)	176 (93%)	13 (7%)	0	100	100
4	H	110/138 (80%)	89 (81%)	19 (17%)	2 (2%)	11	45
4	Q	74/138 (54%)	61 (82%)	13 (18%)	0	100	100
4	Z	15/138 (11%)	11 (73%)	3 (20%)	1 (7%)	1	8
5	1	23/61 (38%)	19 (83%)	3 (13%)	1 (4%)	3	19
5	I	43/61 (70%)	33 (77%)	6 (14%)	4 (9%)	1	4
5	R	30/61 (49%)	25 (83%)	5 (17%)	0	100	100
All	All	9485/10377 (91%)	8800 (93%)	625 (7%)	60 (1%)	30	72

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	101	ILE
5	I	55	GLU
1	L	390	GLY
2	N	221	GLN
2	V	347	ALA

### 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	388/412 (94%)	369 (95%)	19 (5%)	31	71
1	B	388/412 (94%)	373 (96%)	15 (4%)	39	77
1	C	390/412 (95%)	378 (97%)	12 (3%)	47	83
1	J	387/412 (94%)	372 (96%)	15 (4%)	39	77
1	K	390/412 (95%)	372 (95%)	18 (5%)	33	73
1	L	388/412 (94%)	365 (94%)	23 (6%)	24	63
1	S	385/412 (93%)	365 (95%)	20 (5%)	29	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	T	386/412 (94%)	371 (96%)	15 (4%)	39	77
1	U	387/412 (94%)	376 (97%)	11 (3%)	51	84
2	D	379/390 (97%)	362 (96%)	17 (4%)	34	74
2	E	370/390 (95%)	354 (96%)	16 (4%)	35	75
2	F	375/390 (96%)	358 (96%)	17 (4%)	34	74
2	M	378/390 (97%)	360 (95%)	18 (5%)	31	71
2	N	378/390 (97%)	357 (94%)	21 (6%)	26	65
2	O	378/390 (97%)	366 (97%)	12 (3%)	46	82
2	V	379/390 (97%)	364 (96%)	15 (4%)	38	77
2	W	378/390 (97%)	360 (95%)	18 (5%)	31	71
2	X	379/390 (97%)	364 (96%)	15 (4%)	38	77
3	G	226/236 (96%)	210 (93%)	16 (7%)	18	54
3	P	200/236 (85%)	184 (92%)	16 (8%)	15	47
3	Y	164/236 (70%)	150 (92%)	14 (8%)	13	45
4	H	64/112 (57%)	54 (84%)	10 (16%)	3	16
4	Q	11/112 (10%)	9 (82%)	2 (18%)	2	11
5	1	2/48 (4%)	2 (100%)	0	100	100
5	I	28/48 (58%)	25 (89%)	3 (11%)	8	31
5	R	5/48 (10%)	4 (80%)	1 (20%)	1	8
All	All	7583/8294 (91%)	7224 (95%)	359 (5%)	32	72

5 of 359 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	166	ARG
2	N	113	LEU
2	X	22	ASP
1	L	267	LEU
2	M	89	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 70 such sidechains are listed below:

Mol	Chain	Res	Type
1	L	132	GLN

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Mol	Chain	Res	Type
2	N	168	GLN
2	X	328	HIS
1	L	174	GLN
1	L	398	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 30 ligands modelled in this entry, 15 are monoatomic - leaving 15 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
6	ANP	A	600	7	27,33,33	2.15	8 (29%)	30,52,52	2.19	5 (16%)
6	ANP	B	600	7	27,33,33	2.01	7 (25%)	30,52,52	2.38	7 (23%)
6	ANP	C	600	7	27,33,33	2.08	6 (22%)	30,52,52	2.33	7 (23%)
6	ANP	D	600	7	27,33,33	1.90	6 (22%)	30,52,52	2.20	8 (26%)
6	ANP	F	600	7	27,33,33	2.01	6 (22%)	30,52,52	2.33	7 (23%)
6	ANP	J	600	7	27,33,33	1.97	6 (22%)	30,52,52	2.31	6 (20%)
6	ANP	K	600	7	27,33,33	2.06	6 (22%)	30,52,52	2.35	8 (26%)
6	ANP	L	600	7	27,33,33	2.15	8 (29%)	30,52,52	2.26	9 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
6	ANP	M	600	7	27,33,33	1.95	5 (18%)	30,52,52	2.50	6 (20%)
6	ANP	O	600	7	27,33,33	1.96	6 (22%)	30,52,52	2.30	7 (23%)
6	ANP	S	600	7	27,33,33	2.13	7 (25%)	30,52,52	2.25	7 (23%)
6	ANP	T	600	7	27,33,33	2.18	6 (22%)	30,52,52	2.31	7 (23%)
6	ANP	U	600	7	27,33,33	2.06	6 (22%)	30,52,52	2.48	8 (26%)
6	ANP	V	600	7	27,33,33	1.97	6 (22%)	30,52,52	2.43	9 (30%)
6	ANP	X	600	7	27,33,33	1.97	6 (22%)	30,52,52	2.45	8 (26%)

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
6	ANP	A	600	7	-	2/12/38/38	0/3/3/3
6	ANP	B	600	7	-	2/12/38/38	0/3/3/3
6	ANP	C	600	7	-	1/12/38/38	0/3/3/3
6	ANP	D	600	7	-	0/12/38/38	0/3/3/3
6	ANP	F	600	7	-	0/12/38/38	0/3/3/3
6	ANP	J	600	7	-	2/12/38/38	0/3/3/3
6	ANP	K	600	7	-	0/12/38/38	0/3/3/3
6	ANP	L	600	7	-	2/12/38/38	0/3/3/3
6	ANP	M	600	7	-	1/12/38/38	0/3/3/3
6	ANP	O	600	7	-	0/12/38/38	0/3/3/3
6	ANP	S	600	7	-	0/12/38/38	0/3/3/3
6	ANP	T	600	7	-	1/12/38/38	0/3/3/3
6	ANP	U	600	7	-	0/12/38/38	0/3/3/3
6	ANP	V	600	7	-	0/12/38/38	0/3/3/3
6	ANP	X	600	7	-	0/12/38/38	0/3/3/3

The worst 5 of 95 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	L	600	ANP	PG-O2G	-2.54	1.49	1.56
6	A	600	ANP	PG-O2G	-2.49	1.49	1.56
6	L	600	ANP	PG-O3G	-2.16	1.50	1.56
6	D	600	ANP	PB-O2B	-2.13	1.50	1.56
6	V	600	ANP	C2-N3	2.05	1.35	1.32

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	ANP	N3-C2-N1	-7.82	122.91	128.89
6	D	600	ANP	N3-C2-N1	-7.64	123.05	128.89
6	U	600	ANP	N3-C2-N1	-7.50	123.15	128.89
6	M	600	ANP	O1G-PG-N3B	-7.43	100.51	111.90
6	T	600	ANP	N3-C2-N1	-7.39	123.23	128.89

There are no chirality outliers.

5 of 11 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	M	600	ANP	O1G-PG-N3B-PB
6	J	600	ANP	O1B-PB-N3B-PG
6	J	600	ANP	O1G-PG-N3B-PB
6	A	600	ANP	O1G-PG-N3B-PB
6	C	600	ANP	O1B-PB-N3B-PG

There are no ring outliers.

12 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	600	ANP	1	0
6	B	600	ANP	4	0
6	F	600	ANP	1	0
6	J	600	ANP	1	0
6	K	600	ANP	3	0
6	L	600	ANP	1	0
6	M	600	ANP	4	0
6	O	600	ANP	3	0
6	T	600	ANP	1	0
6	U	600	ANP	1	0
6	V	600	ANP	1	0
6	X	600	ANP	4	0

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	482/510 (94%)	-0.48	0 100 100	41, 63, 99, 156	0
1	B	483/510 (94%)	-0.21	3 (0%) 90 73	48, 92, 148, 188	0
1	C	484/510 (94%)	-0.39	0 100 100	43, 73, 129, 177	0
1	J	481/510 (94%)	-0.24	2 (0%) 93 80	60, 100, 149, 206	0
1	K	486/510 (95%)	-0.04	16 (3%) 50 22	78, 126, 187, 217	0
1	L	482/510 (94%)	-0.39	0 100 100	47, 68, 137, 194	0
1	S	478/510 (93%)	-0.19	10 (2%) 67 36	77, 109, 153, 179	0
1	T	479/510 (93%)	0.24	31 (6%) 22 8	103, 151, 186, 202	0
1	U	481/510 (94%)	0.22	32 (6%) 21 7	104, 150, 181, 217	0
2	D	470/484 (97%)	-0.42	1 (0%) 95 87	42, 70, 123, 181	0
2	E	468/484 (96%)	-0.21	10 (2%) 67 36	46, 86, 161, 211	0
2	F	469/484 (96%)	-0.29	1 (0%) 95 87	48, 89, 129, 169	0
2	M	470/484 (97%)	-0.30	3 (0%) 90 73	55, 86, 134, 180	0
2	N	470/484 (97%)	0.09	19 (4%) 42 17	71, 133, 199, 229	0
2	O	468/484 (96%)	-0.29	0 100 100	54, 94, 141, 175	0
2	V	470/484 (97%)	0.13	28 (5%) 25 9	93, 138, 180, 210	0
2	W	467/484 (96%)	-0.05	18 (3%) 43 18	89, 117, 164, 189	0
2	X	469/484 (96%)	0.08	21 (4%) 37 15	93, 134, 185, 234	0
3	G	266/278 (95%)	-0.23	2 (0%) 87 67	63, 103, 140, 167	0
3	P	246/278 (88%)	0.25	14 (5%) 27 10	69, 131, 195, 237	0
3	Y	201/278 (72%)	0.46	20 (9%) 9 4	107, 146, 192, 232	0
4	H	116/138 (84%)	-0.03	6 (5%) 31 12	82, 127, 216, 236	0
4	Q	84/138 (60%)	0.03	4 (4%) 34 14	109, 150, 208, 214	0
4	Z	17/138 (12%)	2.27	11 (64%) 0 0	190, 210, 236, 245	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
5	1	27/61 (44%)	1.60	9 (33%) 0 0	159, 168, 187, 210	0
5	I	49/61 (80%)	-0.06	2 (4%) 41 16	97, 127, 178, 217	0
5	R	34/61 (55%)	-0.32	1 (2%) 55 26	108, 122, 187, 200	0
All	All	9597/10377 (92%)	-0.12	264 (2%) 56 27	41, 108, 176, 245	0

The worst 5 of 264 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	U	26	ASN	6.4
1	T	491	LEU	5.5
2	X	7	THR	5.3
5	1	33	SER	5.1
2	X	90	GLU	4.9

## 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(Å <sup>2</sup> )	Q<0.9
7	MG	F	700	1/1	0.97	0.33	5.27	55,55,55,55	0
7	MG	M	700	1/1	0.92	0.35	5.03	53,53,53,53	0
7	MG	D	700	1/1	0.94	0.29	4.72	48,48,48,48	0
6	ANP	C	600	31/31	0.96	0.20	0.54	57,68,75,75	0
6	ANP	D	600	31/31	0.98	0.19	0.34	55,65,68,69	0
6	ANP	M	600	31/31	0.98	0.20	0.19	60,70,73,74	0
6	ANP	A	600	31/31	0.98	0.19	0.16	44,57,61,63	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
6	ANP	L	600	31/31	0.96	0.19	0.00	49,62,70,70	0
6	ANP	K	600	31/31	0.91	0.19	-0.06	79,96,100,101	0
6	ANP	F	600	31/31	0.96	0.20	-0.23	65,79,84,85	0
6	ANP	J	600	31/31	0.94	0.17	-0.24	60,74,82,83	0
6	ANP	V	600	31/31	0.95	0.20	-0.42	80,100,102,102	0
7	MG	V	700	1/1	0.97	0.21	-0.48	61,61,61,61	0
6	ANP	U	600	31/31	0.89	0.20	-0.48	73,79,82,82	0
6	ANP	T	600	31/31	0.92	0.17	-0.52	81,102,107,108	0
6	ANP	B	600	31/31	0.95	0.16	-0.71	66,79,81,82	0
6	ANP	O	600	31/31	0.97	0.18	-0.75	69,79,81,82	0
6	ANP	S	600	31/31	0.96	0.14	-0.89	64,78,80,80	0
6	ANP	X	600	31/31	0.96	0.17	-1.15	83,95,97,97	0
7	MG	O	700	1/1	0.95	0.11	-3.73	61,61,61,61	0
7	MG	X	700	1/1	0.98	0.15	-5.66	70,70,70,70	0
7	MG	K	700	1/1	0.97	0.19	-	66,66,66,66	0
7	MG	L	700	1/1	0.95	0.33	-	48,48,48,48	0
7	MG	S	700	1/1	0.96	0.27	-	53,53,53,53	0
7	MG	C	700	1/1	0.97	0.37	-	52,52,52,52	0
7	MG	A	700	1/1	0.98	0.32	-	41,41,41,41	0
7	MG	B	700	1/1	0.98	0.32	-	57,57,57,57	0
7	MG	U	700	1/1	0.99	0.30	-	61,61,61,61	0
7	MG	J	700	1/1	0.88	0.24	-	51,51,51,51	0
7	MG	T	700	1/1	0.93	0.28	-	62,62,62,62	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.