wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 11:25 AM GMT

PDB ID	:	3OFN
Title	:	Structure of four mutant forms of yeast F1 ATPase: alpha-N67I
Authors	:	Arsenieva, D.; Symersky, J.; Wang, Y.; Pagadala, V.; Mueller, D.M.
Deposited on	:	2010-08-15
Resolution	:	3.20 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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

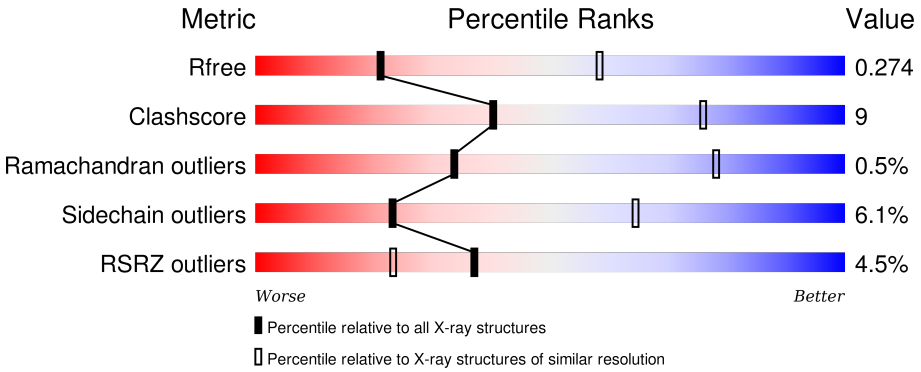
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.20 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	1124 (3.24-3.16)
Clashscore	102246	1024 (3.22-3.18)
Ramachandran outliers	100387	1004 (3.22-3.18)
Sidechain outliers	100360	1003 (3.22-3.18)
RSRZ outliers	91569	1129 (3.24-3.16)

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 >=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 <=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	69% 24% • 5%
1	B	510	3% 72% 22% • 5%
1	C	510	2% 78% 15% • 5%
1	J	510	4% 74% 19% • 5%
1	K	510	7% 74% 21% 5%

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Mol	Chain	Length	Quality of chain
1	L	510	3% 71% 22% 6%
1	S	510	% 76% 17% 5%
1	T	510	% 75% 19% 5%
1	U	510	5% 76% 18% 5%
2	D	484	2% 74% 22%
2	E	484	3% 70% 24%
2	F	484	2% 73% 24%
2	M	484	5% 69% 24% 5%
2	N	484	10% 69% 25%
2	O	484	6% 78% 18%
2	V	484	6% 53% 20% 26%
2	W	484	% 77% 18%
2	X	484	% 76% 21%
3	G	278	67% 28%
3	P	278	15% 71% 24%
3	Y	278	11% 30% 11% 59%
4	H	138	64% 20% 12%
4	Q	138	27% 64% 9% 27%
5	I	61	2% 61% 21% 8% 10%
5	R	61	8% 70% 20% 10%

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
7	MG	O	700	-	-	-	X
7	MG	X	700	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 70481 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	485	Total	C	N	O	S	0	0	0
			3691	2336	650	702	3			
1	B	486	Total	C	N	O	S	0	0	0
			3690	2336	648	703	3			
1	C	484	Total	C	N	O	S	0	0	0
			3680	2327	649	701	3			
1	J	482	Total	C	N	O	S	0	0	0
			3664	2316	647	698	3			
1	K	483	Total	C	N	O	S	0	0	0
			3578	2255	634	686	3			
1	L	479	Total	C	N	O	S	0	0	0
			3608	2282	637	686	3			
1	S	483	Total	C	N	O	S	0	0	0
			3642	2302	640	697	3			
1	T	484	Total	C	N	O	S	0	0	0
			3639	2296	642	698	3			
1	U	485	Total	C	N	O	S	0	0	0
			3511	2205	619	684	3			

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	ILE	ASN	ENGINEERED MUTATION	UNP P07251
B	67	ILE	ASN	ENGINEERED MUTATION	UNP P07251
C	67	ILE	ASN	ENGINEERED MUTATION	UNP P07251
J	67	ILE	ASN	ENGINEERED MUTATION	UNP P07251
K	67	ILE	ASN	ENGINEERED MUTATION	UNP P07251
L	67	ILE	ASN	ENGINEERED MUTATION	UNP P07251
S	67	ILE	ASN	ENGINEERED MUTATION	UNP P07251
T	67	ILE	ASN	ENGINEERED MUTATION	UNP P07251
U	67	ILE	ASN	ENGINEERED MUTATION	UNP P07251

- 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
			3545	2248	603	688	6			
2	E	469	Total	C	N	O	S	0	0	0
			3511	2226	598	681	6			
2	F	469	Total	C	N	O	S	0	0	0
			3539	2245	603	685	6			
2	M	460	Total	C	N	O	S	0	0	0
			3436	2180	584	667	5			
2	N	463	Total	C	N	O	S	0	0	0
			3403	2160	573	665	5			
2	O	469	Total	C	N	O	S	0	0	0
			3449	2191	581	671	6			
2	V	360	Total	C	N	O	S	0	0	0
			2582	1625	439	515	3			
2	W	468	Total	C	N	O	S	0	0	0
			3468	2198	590	674	6			
2	X	469	Total	C	N	O	S	0	0	0
			3447	2181	588	673	5			

There are 72 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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
F	1	HIS	-	EXPRESSION TAG	UNP P00830
F	2	HIS	-	EXPRESSION TAG	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
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
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
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
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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
X	-5	ALA	-	EXPRESSION TAG	UNP P00830
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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	268	Total	C	N	O	S	0	0	0
			2064	1297	358	399	10			
3	P	268	Total	C	N	O	S	0	0	0
			1869	1163	320	380	6			
3	Y	115	Total	C	N	O	S	0	0	0
			790	482	141	163	4			

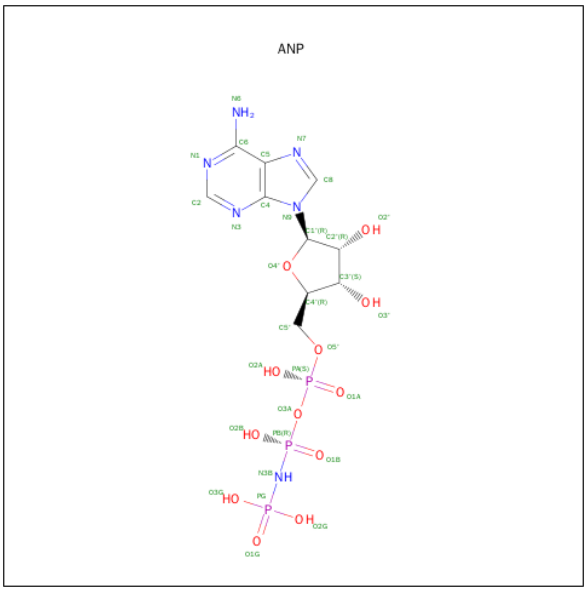
- Molecule 4 is a protein called ATP synthase subunit delta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	122	Total	C	N	O	S	0	0	0
			815	513	139	161	2			
4	Q	101	Total	C	N	O	S	0	0	0
			625	389	110	125	1			

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	55	Total	C	N	O	0	0	0
			388	242	68	78			
5	R	55	Total	C	N	O	0	0	0
			367	227	66	74			

- Molecule 6 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	J	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	K	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	L	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	M	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	O	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	S	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	T	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	U	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
6	V	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

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

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

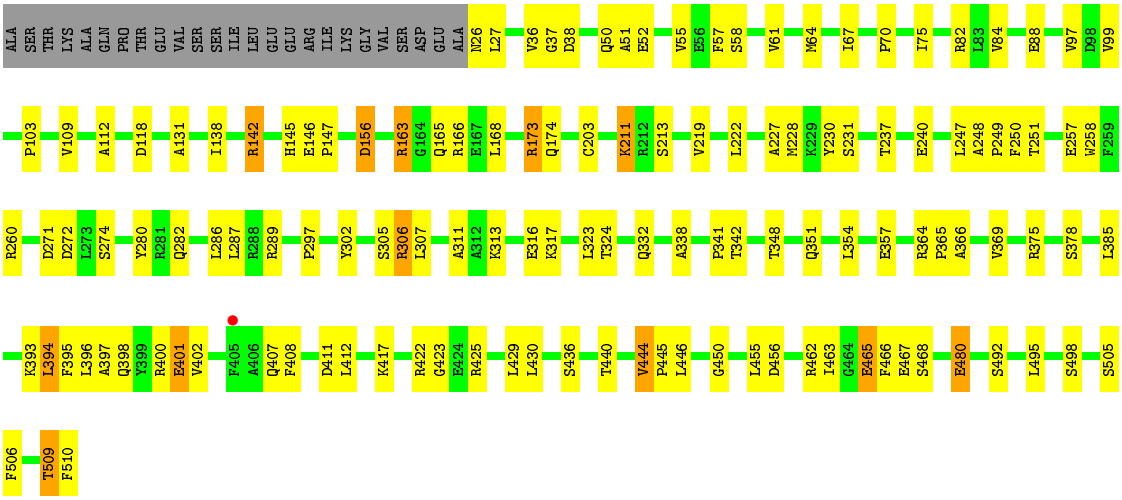
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total 1	Mg 1	0	0
7	D	1	Total 1	Mg 1	0	0
7	K	1	Total 1	Mg 1	0	0
7	B	1	Total 1	Mg 1	0	0
7	C	1	Total 1	Mg 1	0	0
7	V	1	Total 1	Mg 1	0	0
7	A	1	Total 1	Mg 1	0	0
7	T	1	Total 1	Mg 1	0	0
7	U	1	Total 1	Mg 1	0	0
7	X	1	Total 1	Mg 1	0	0
7	O	1	Total 1	Mg 1	0	0
7	L	1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

3 Residue-property plots (i)

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.

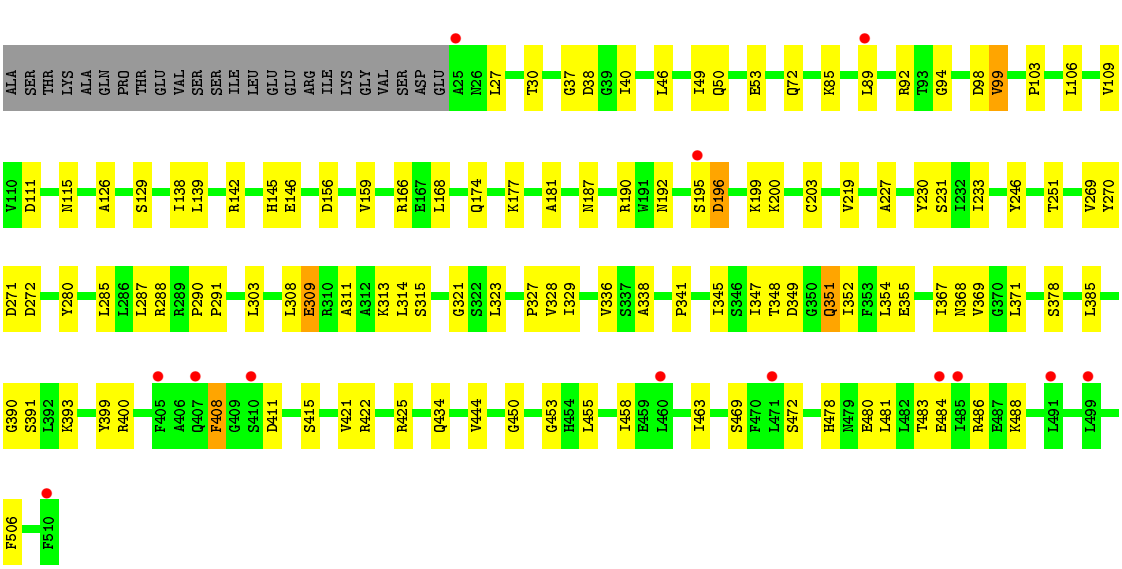
- Molecule 1: ATP synthase subunit alpha

Chain A:



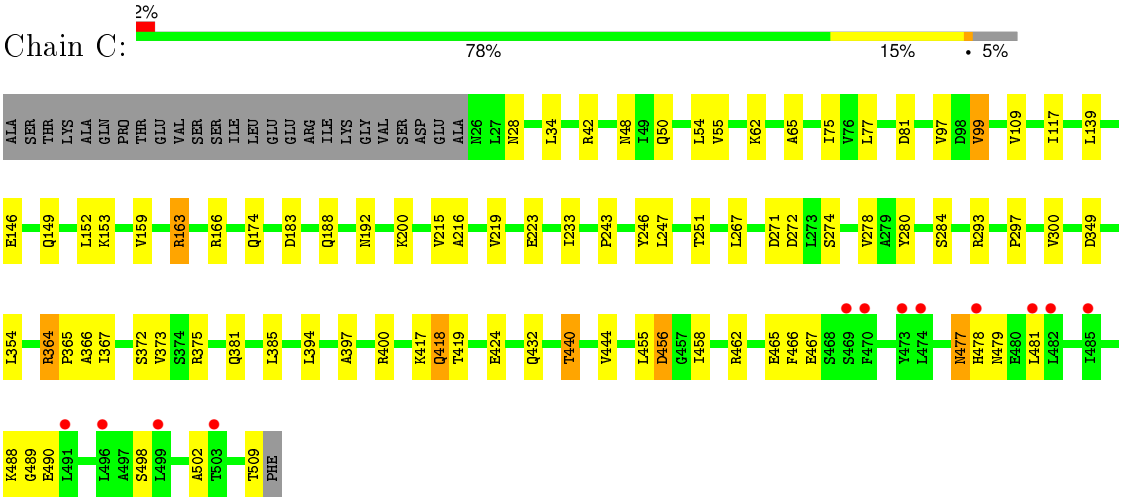
- Molecule 1: ATP synthase subunit alpha

Chain B:



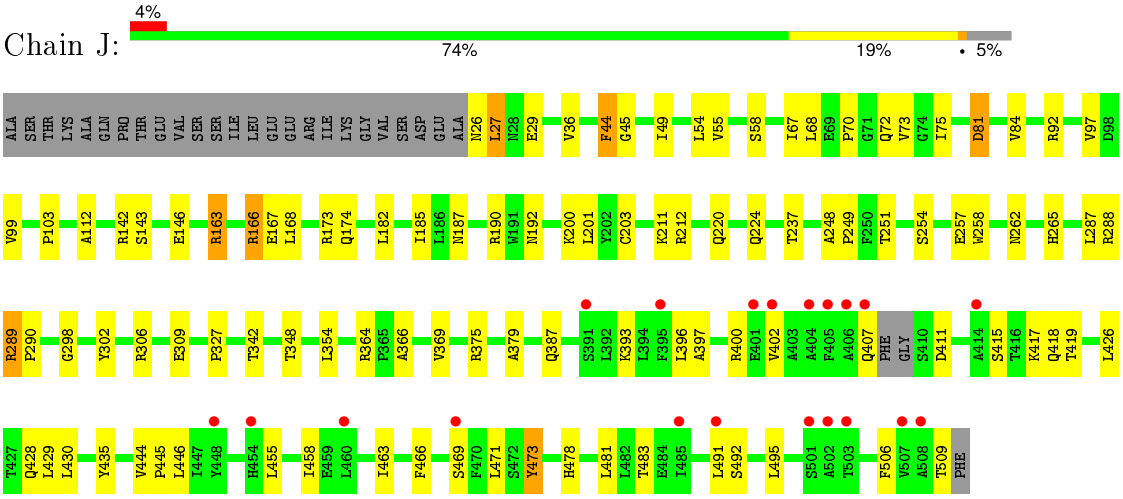
• Molecule 1: ATP synthase subunit alpha

Chain C:



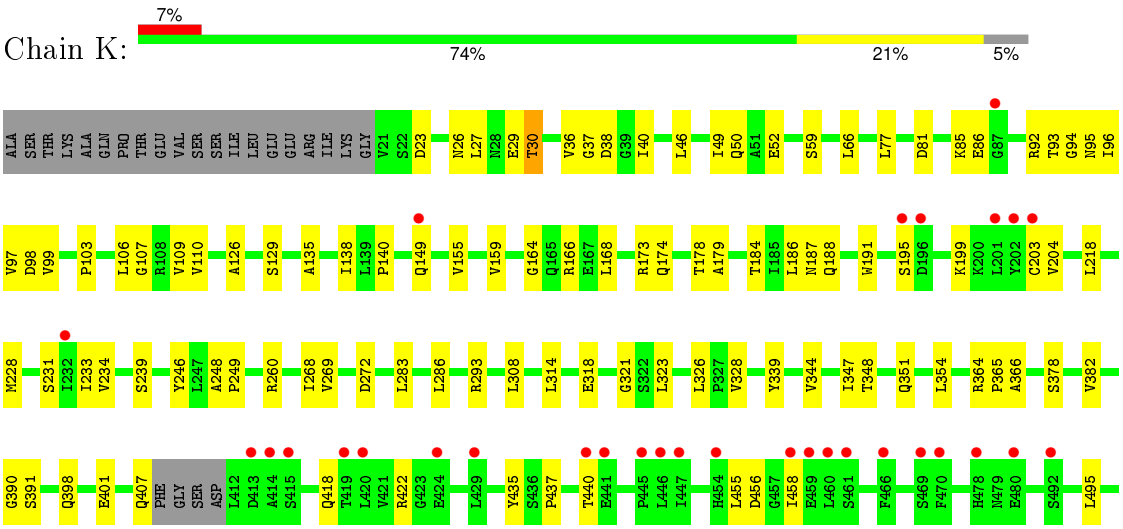
• Molecule 1: ATP synthase subunit alpha

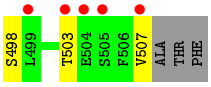
Chain J:



• Molecule 1: ATP synthase subunit alpha

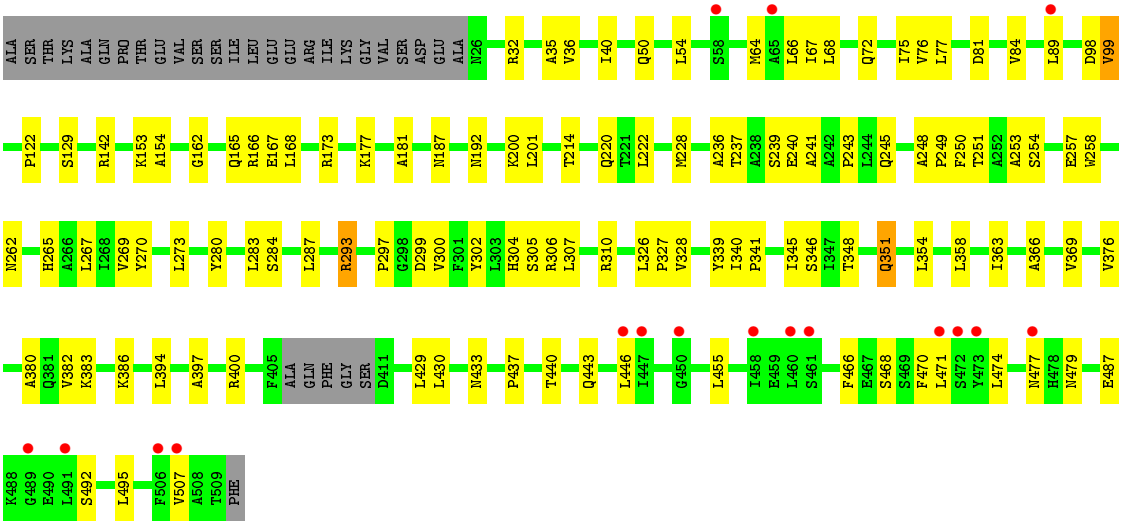
Chain K:





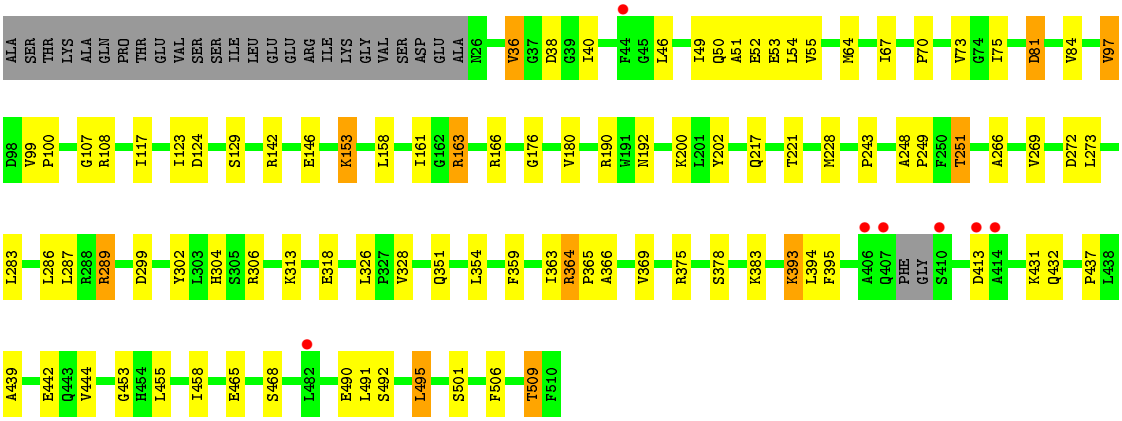
• Molecule 1: ATP synthase subunit alpha

Chain L:



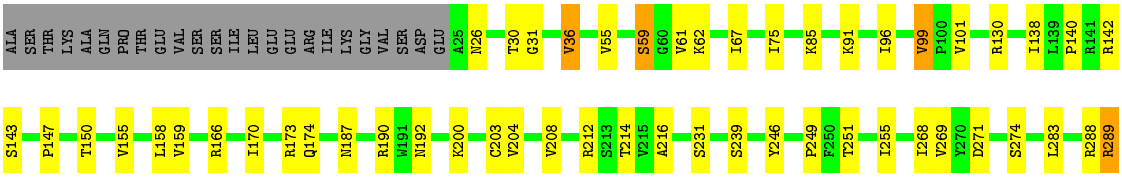
• Molecule 1: ATP synthase subunit alpha

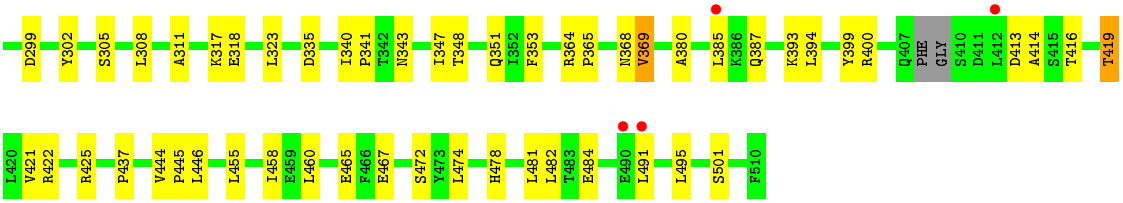
Chain S:



• Molecule 1: ATP synthase subunit alpha

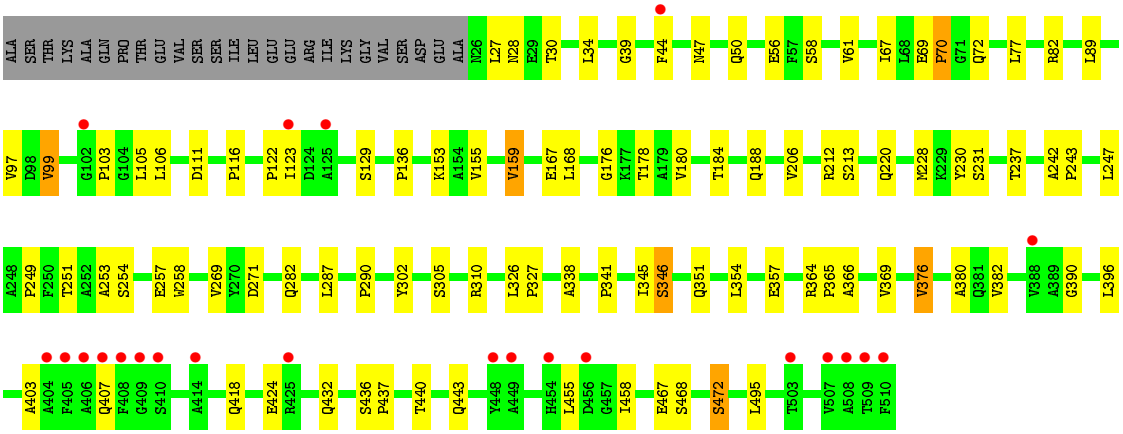
Chain T:





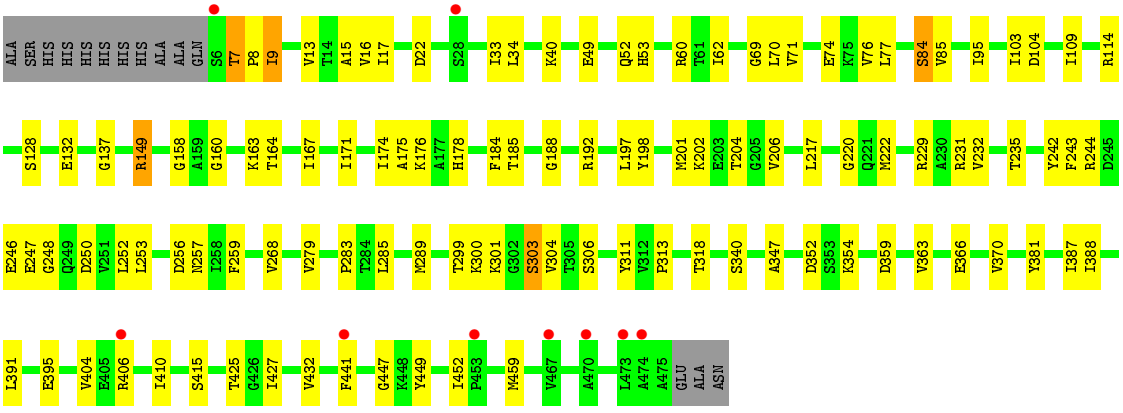
• Molecule 1: ATP synthase subunit alpha

Chain U:



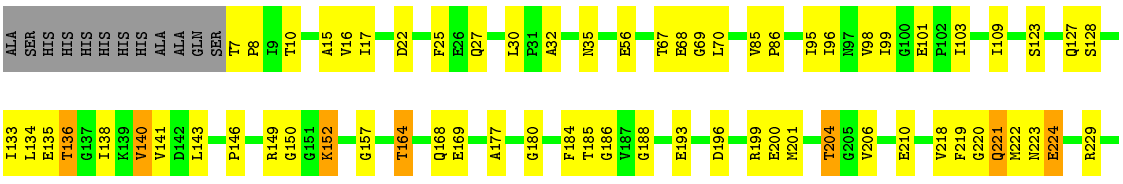
• Molecule 2: ATP synthase subunit beta

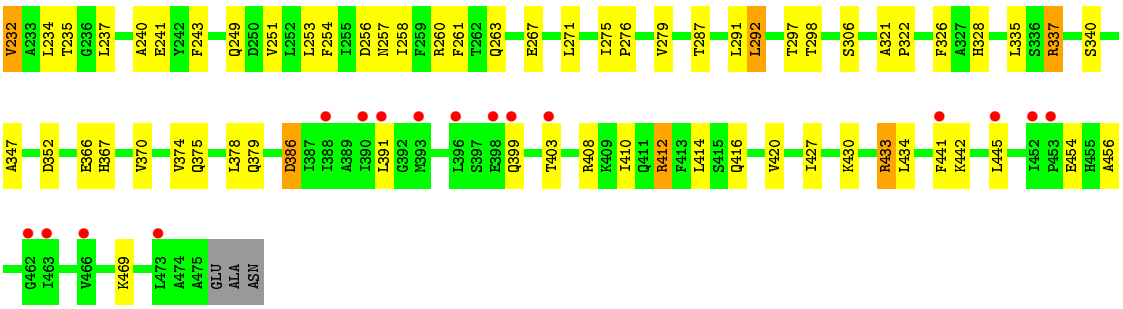
Chain D:



• Molecule 2: ATP synthase subunit beta

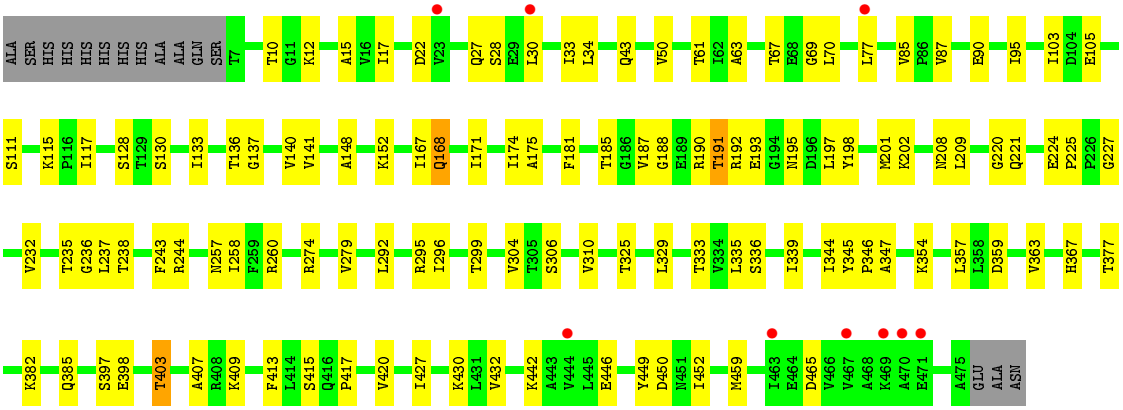
Chain E:





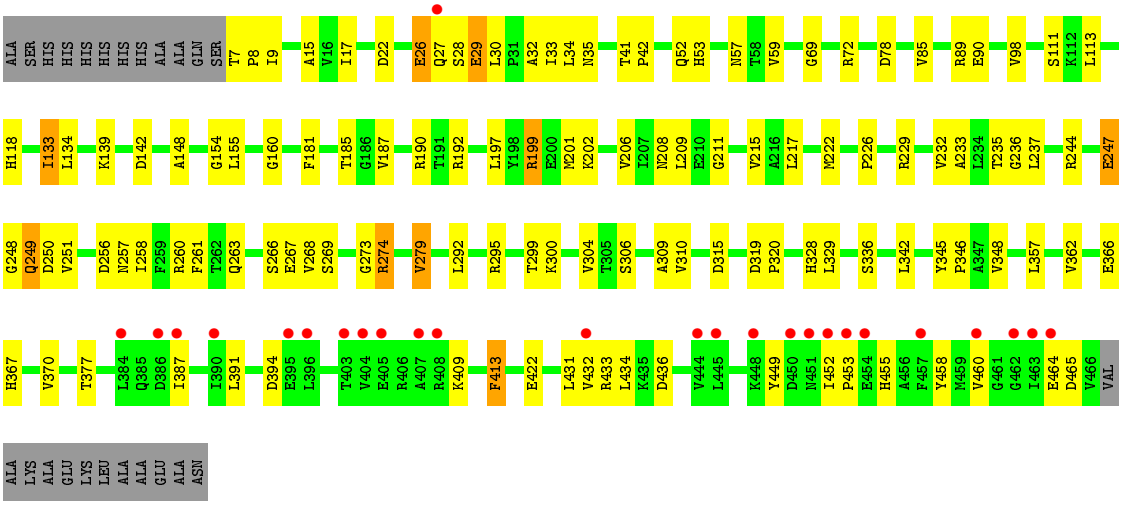
• Molecule 2: ATP synthase subunit beta

Chain F:



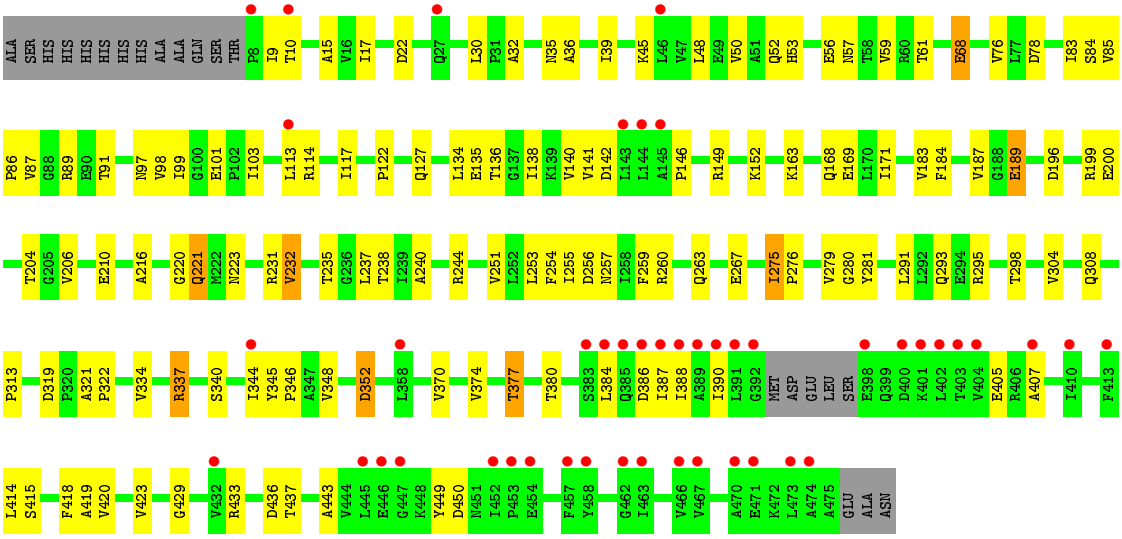
• Molecule 2: ATP synthase subunit beta

Chain M:



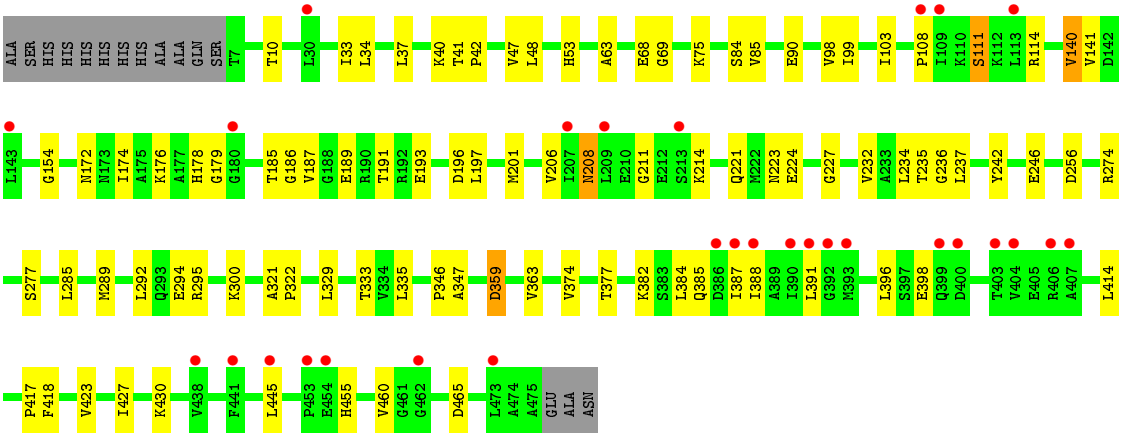
• Molecule 2: ATP synthase subunit beta

Chain N:



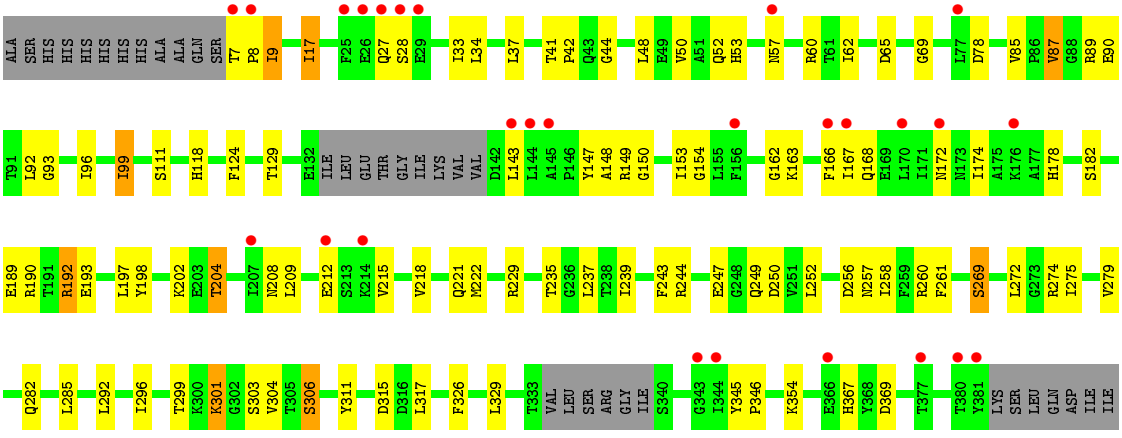
• Molecule 2: ATP synthase subunit beta

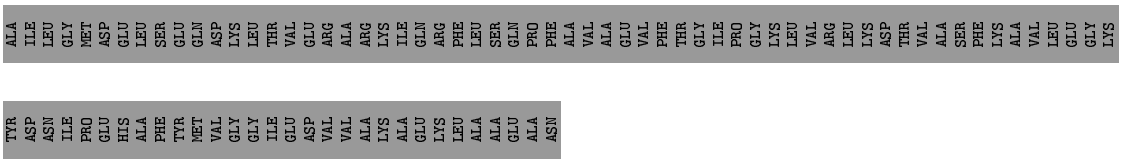
Chain O:



• Molecule 2: ATP synthase subunit beta

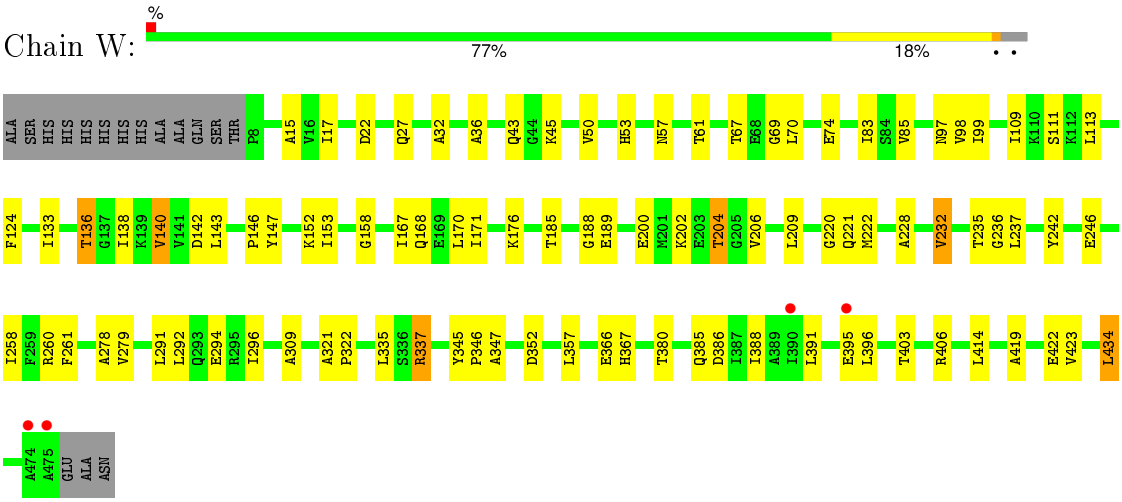
Chain V:





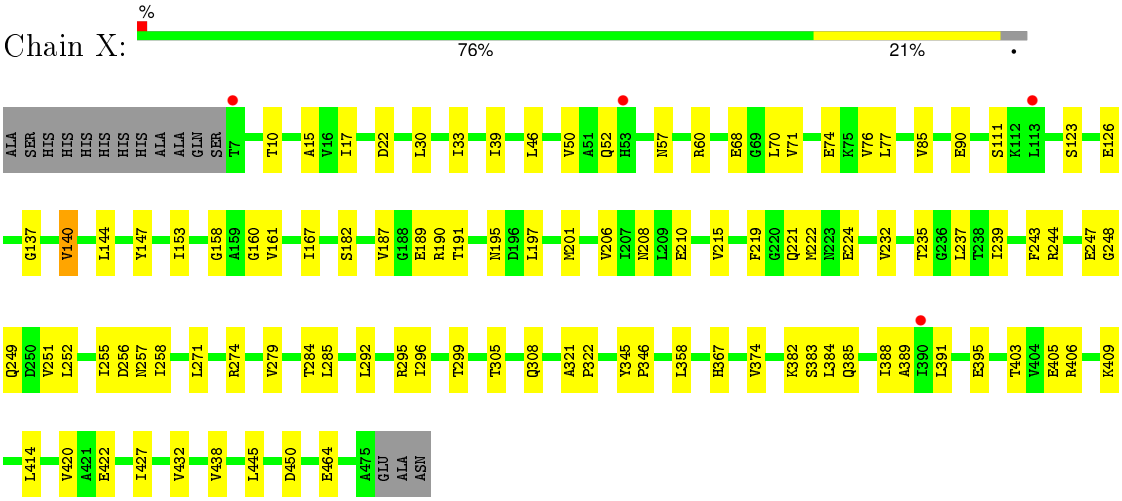
• Molecule 2: ATP synthase subunit beta

Chain W:



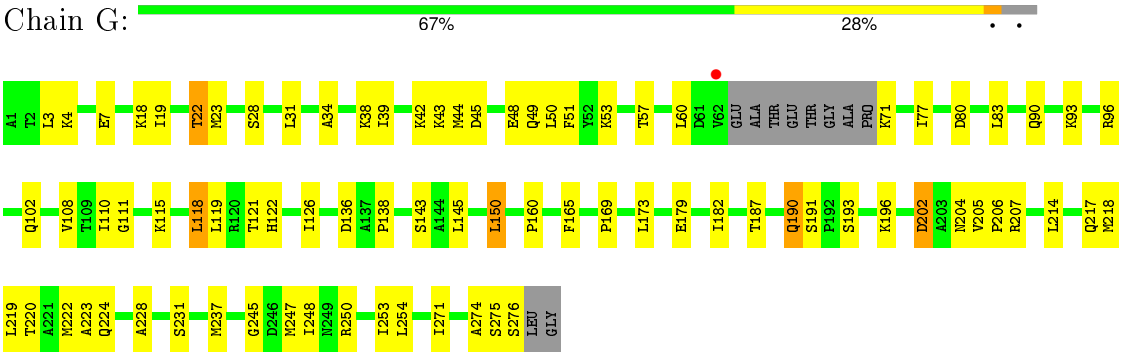
• Molecule 2: ATP synthase subunit beta

Chain X:



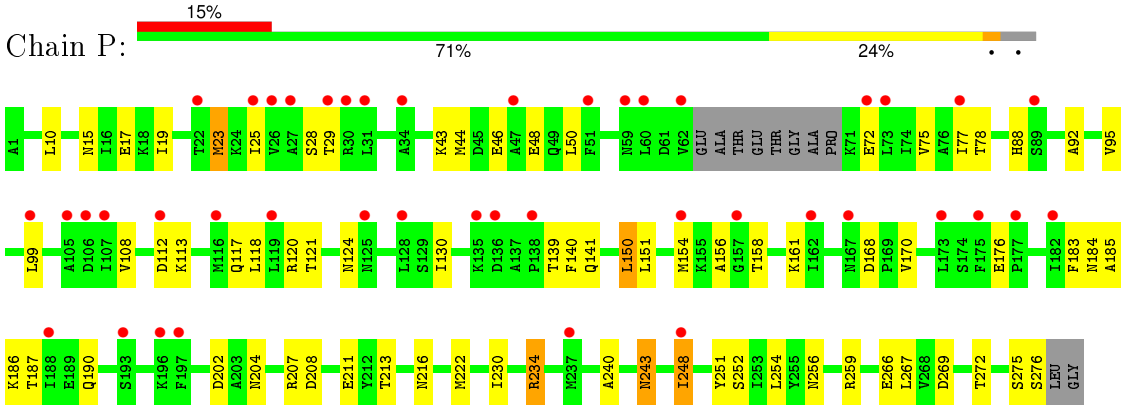
• Molecule 3: ATP synthase subunit gamma

Chain G:



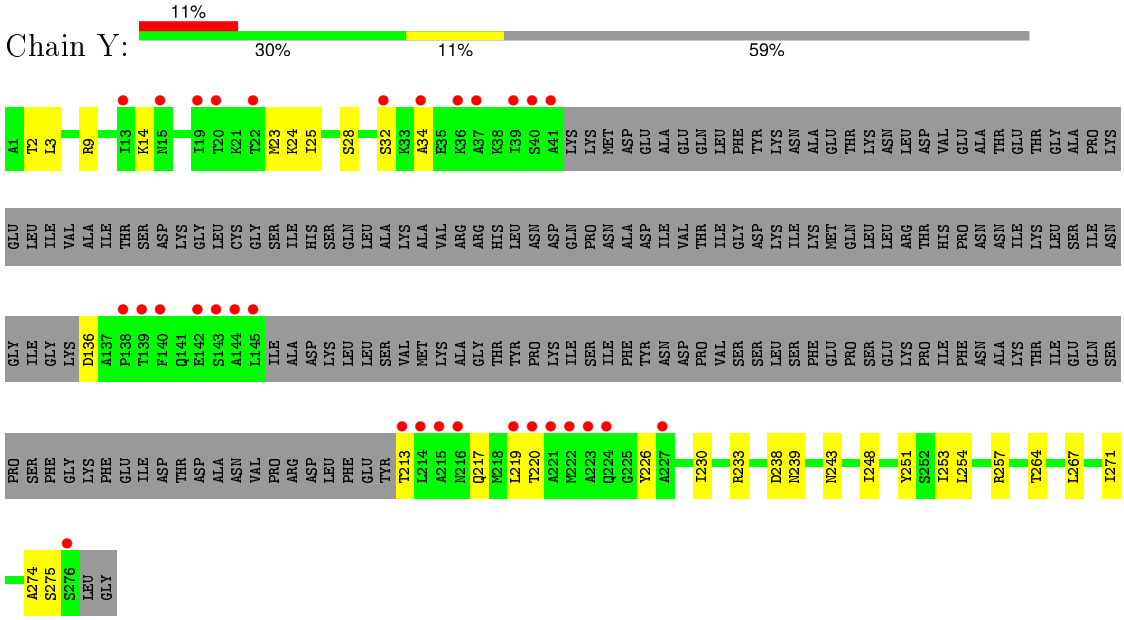
- Molecule 3: ATP synthase subunit gamma

Chain P:



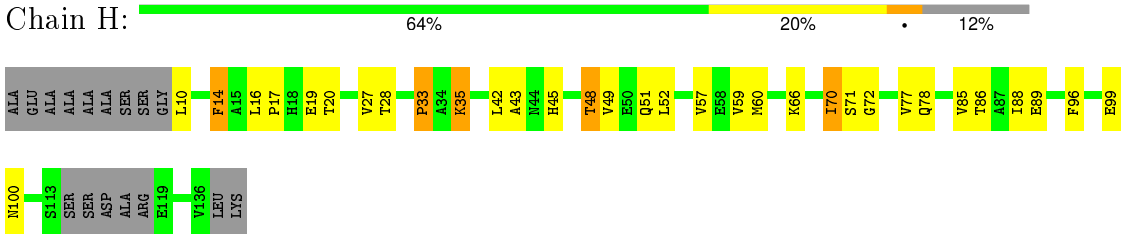
- Molecule 3: ATP synthase subunit gamma

Chain Y:



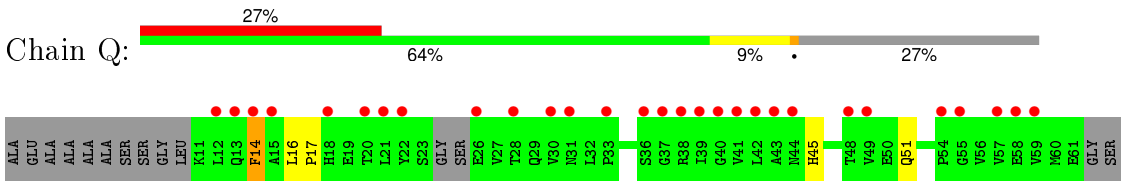
- Molecule 4: ATP synthase subunit delta

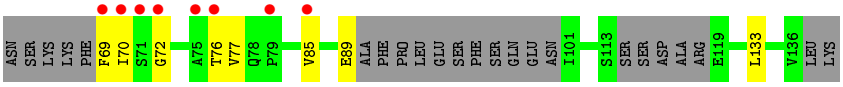
Chain H:



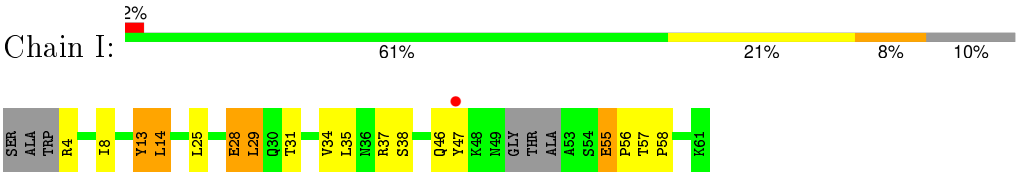
- Molecule 4: ATP synthase subunit delta

Chain Q:

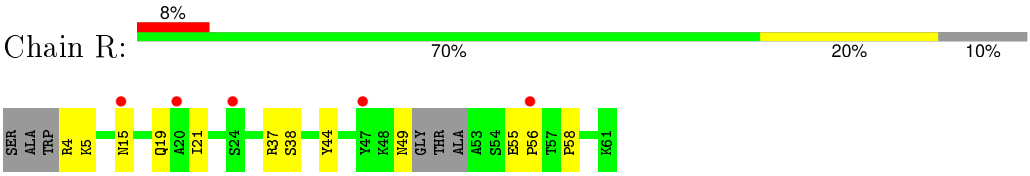




• Molecule 5: ATP synthase subunit epsilon



• Molecule 5: ATP synthase subunit epsilon



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	112.02Å 290.62Å 188.47Å 90.00° 102.34° 90.00°	Depositor
Resolution (Å)	50.00 – 3.20 49.63 – 3.20	Depositor EDS
% Data completeness (in resolution range)	91.2 (50.00-3.20) 91.2 (49.63-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.4.0066	Depositor
R, R_{free}	0.210 , 0.276 0.211 , 0.274	Depositor DCC
R_{free} test set	3554 reflections (2.05%)	DCC
Wilson B-factor (Å^2)	90.9	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 61.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.30$	Xtriage
Outliers	2 of 176635 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	70481	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.82% 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, 0.375 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

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	0.43	0/3748	0.60	0/5073
1	B	0.40	0/3747	0.57	0/5073
1	C	0.41	0/3736	0.57	0/5057
1	J	0.39	0/3718	0.56	0/5032
1	K	0.37	0/3630	0.53	0/4926
1	L	0.40	0/3662	0.57	0/4963
1	S	0.41	0/3696	0.57	0/5008
1	T	0.39	0/3693	0.57	0/5006
1	U	0.37	0/3564	0.53	0/4850
2	D	0.41	0/3601	0.57	0/4884
2	E	0.43	0/3567	0.57	0/4846
2	F	0.40	0/3595	0.59	0/4876
2	M	0.42	0/3492	0.57	0/4747
2	N	0.38	0/3457	0.56	0/4708
2	O	0.38	0/3505	0.56	0/4774
2	V	0.42	0/2623	0.56	0/3585
2	W	0.43	0/3524	0.59	0/4796
2	X	0.39	0/3503	0.56	0/4774
3	G	0.39	0/2089	0.58	0/2812
3	P	0.36	0/1892	0.50	0/2586
3	Y	0.39	0/791	0.54	0/1077
4	H	0.45	0/827	0.63	0/1133
4	Q	0.40	0/629	0.50	0/866
5	I	0.48	0/393	0.69	0/537
5	R	0.45	0/372	0.51	0/510
All	All	0.40	0/71054	0.57	0/96499

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3691	0	3777	84	0
1	B	3690	0	3771	66	0
1	C	3680	0	3768	47	0
1	J	3664	0	3752	68	0
1	K	3578	0	3577	59	0
1	L	3608	0	3668	66	0
1	S	3642	0	3697	58	0
1	T	3639	0	3673	63	0
1	U	3511	0	3411	49	0
2	D	3545	0	3614	64	0
2	E	3511	0	3549	80	0
2	F	3539	0	3611	68	0
2	M	3436	0	3459	78	0
2	N	3403	0	3385	77	0
2	O	3449	0	3435	52	0
2	V	2582	0	2492	67	0
2	W	3468	0	3463	59	0
2	X	3447	0	3402	61	0
3	G	2064	0	2125	46	0
3	P	1869	0	1710	36	0
3	Y	790	0	735	17	0
4	H	815	0	712	26	0
4	Q	625	0	501	6	0
5	I	388	0	344	18	0
5	R	367	0	301	8	0
6	A	31	0	13	0	0
6	B	31	0	13	2	0
6	C	31	0	13	3	0
6	D	31	0	13	2	0
6	F	31	0	13	3	0
6	J	31	0	13	3	0
6	K	31	0	13	1	0
6	L	31	0	13	0	0
6	M	31	0	13	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	O	31	0	13	0	0
6	S	31	0	13	0	0
6	T	31	0	13	2	0
6	U	31	0	13	0	0
6	V	31	0	13	2	0
6	X	31	0	13	2	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	70481	0	70127	1222	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 9.

The worst 5 of 1222 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)
6:F:600:ANP:H8	6:F:600:ANP:H5'1	1.26	1.16
3:G:96:ARG:HE	3:G:121:THR:HG21	1.25	1.01
2:D:85:VAL:HG11	2:D:235:THR:HG23	1.42	1.00
5:I:31:THR:HG22	5:I:34:VAL:HG23	1.45	0.98
1:T:289:ARG:HH11	1:T:289:ARG:HG2	1.23	0.98

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	483/510 (95%)	457 (95%)	25 (5%)	1 (0%)	52 88
1	B	484/510 (95%)	455 (94%)	25 (5%)	4 (1%)	24 69
1	C	482/510 (94%)	458 (95%)	23 (5%)	1 (0%)	52 88
1	J	478/510 (94%)	443 (93%)	32 (7%)	3 (1%)	30 75
1	K	479/510 (94%)	442 (92%)	37 (8%)	0	100 100
1	L	475/510 (93%)	442 (93%)	31 (6%)	2 (0%)	39 80
1	S	479/510 (94%)	458 (96%)	20 (4%)	1 (0%)	52 88
1	T	480/510 (94%)	454 (95%)	26 (5%)	0	100 100
1	U	483/510 (95%)	450 (93%)	31 (6%)	2 (0%)	39 80
2	D	468/484 (97%)	440 (94%)	26 (6%)	2 (0%)	39 80
2	E	467/484 (96%)	437 (94%)	28 (6%)	2 (0%)	39 80
2	F	467/484 (96%)	443 (95%)	24 (5%)	0	100 100
2	M	458/484 (95%)	421 (92%)	34 (7%)	3 (1%)	26 72
2	N	459/484 (95%)	422 (92%)	34 (7%)	3 (1%)	26 72
2	O	467/484 (96%)	433 (93%)	33 (7%)	1 (0%)	52 88
2	V	354/484 (73%)	318 (90%)	31 (9%)	5 (1%)	14 57
2	W	466/484 (96%)	435 (93%)	30 (6%)	1 (0%)	52 88
2	X	467/484 (96%)	430 (92%)	35 (8%)	2 (0%)	39 80
3	G	264/278 (95%)	249 (94%)	14 (5%)	1 (0%)	39 80
3	P	264/278 (95%)	243 (92%)	19 (7%)	2 (1%)	24 69
3	Y	109/278 (39%)	102 (94%)	7 (6%)	0	100 100
4	H	118/138 (86%)	98 (83%)	17 (14%)	3 (2%)	7 41
4	Q	91/138 (66%)	81 (89%)	10 (11%)	0	100 100
5	I	51/61 (84%)	44 (86%)	3 (6%)	4 (8%)	1 8
5	R	51/61 (84%)	43 (84%)	7 (14%)	1 (2%)	9 48

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	9344/10178 (92%)	8698 (93%)	602 (6%)	44 (0%)	34 78

5 of 44 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	99	GLU
5	I	55	GLU
2	M	27	GLN
5	R	58	PRO
4	H	33	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	391/412 (95%)	361 (92%)	30 (8%)	16 54
1	B	390/412 (95%)	369 (95%)	21 (5%)	27 68
1	C	390/412 (95%)	369 (95%)	21 (5%)	27 68
1	J	388/412 (94%)	367 (95%)	21 (5%)	27 68
1	K	366/412 (89%)	348 (95%)	18 (5%)	31 72
1	L	378/412 (92%)	359 (95%)	19 (5%)	30 71
1	S	382/412 (93%)	357 (94%)	25 (6%)	21 61
1	T	379/412 (92%)	353 (93%)	26 (7%)	19 59
1	U	348/412 (84%)	329 (94%)	19 (6%)	27 68
2	D	379/390 (97%)	362 (96%)	17 (4%)	34 74
2	E	371/390 (95%)	345 (93%)	26 (7%)	19 58
2	F	378/390 (97%)	358 (95%)	20 (5%)	28 69
2	M	363/390 (93%)	339 (93%)	24 (7%)	21 61
2	N	352/390 (90%)	330 (94%)	22 (6%)	22 63
2	O	357/390 (92%)	339 (95%)	18 (5%)	30 71
2	V	261/390 (67%)	246 (94%)	15 (6%)	25 67

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	W	361/390 (93%)	343 (95%)	18 (5%)	30 71
2	X	354/390 (91%)	342 (97%)	12 (3%)	44 80
3	G	226/236 (96%)	206 (91%)	20 (9%)	12 45
3	P	178/236 (75%)	160 (90%)	18 (10%)	9 36
3	Y	72/236 (30%)	64 (89%)	8 (11%)	8 32
4	H	71/112 (63%)	62 (87%)	9 (13%)	5 25
4	Q	46/112 (41%)	43 (94%)	3 (6%)	21 61
5	I	34/48 (71%)	27 (79%)	7 (21%)	1 7
5	R	28/48 (58%)	26 (93%)	2 (7%)	18 57
All	All	7243/8246 (88%)	6804 (94%)	439 (6%)	23 64

5 of 439 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	K	129	SER
2	M	377	THR
2	W	140	VAL
1	K	351	GLN
1	L	351	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 62 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	477	ASN
2	M	52	GLN
2	W	168	GLN
1	L	351	GLN
2	M	195	ASN

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	1.93	7 (25%)	30,52,52	2.28	8 (26%)
6	ANP	B	600	7	27,33,33	2.04	7 (25%)	30,52,52	2.21	8 (26%)
6	ANP	C	600	7	27,33,33	2.05	7 (25%)	30,52,52	2.40	8 (26%)
6	ANP	D	600	7	27,33,33	2.03	7 (25%)	30,52,52	2.13	8 (26%)
6	ANP	F	600	7	27,33,33	2.05	6 (22%)	30,52,52	2.02	7 (23%)
6	ANP	J	600	7	27,33,33	1.97	6 (22%)	30,52,52	2.41	8 (26%)
6	ANP	K	600	7	27,33,33	2.15	6 (22%)	30,52,52	2.16	8 (26%)
6	ANP	L	600	7	27,33,33	1.97	5 (18%)	30,52,52	2.27	8 (26%)
6	ANP	M	600	7	27,33,33	1.96	7 (25%)	30,52,52	2.55	8 (26%)
6	ANP	O	600	7	27,33,33	2.08	9 (33%)	30,52,52	2.20	8 (26%)
6	ANP	S	600	7	27,33,33	2.11	6 (22%)	30,52,52	2.34	6 (20%)
6	ANP	T	600	7	27,33,33	2.09	8 (29%)	30,52,52	2.25	7 (23%)
6	ANP	U	600	7	27,33,33	2.05	7 (25%)	30,52,52	2.23	7 (23%)
6	ANP	V	600	7	27,33,33	2.39	7 (25%)	30,52,52	2.39	6 (20%)
6	ANP	X	600	7	27,33,33	1.79	6 (22%)	30,52,52	2.70	9 (30%)

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	-	1/12/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ANP	B	600	7	-	1/12/38/38	0/3/3/3
6	ANP	C	600	7	-	2/12/38/38	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	-	1/12/38/38	0/3/3/3
6	ANP	L	600	7	-	0/12/38/38	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 101 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	600	ANP	PG-O3G	-2.34	1.50	1.56
6	A	600	ANP	PG-O3G	-2.31	1.50	1.56
6	A	600	ANP	PG-O2G	-2.30	1.50	1.56
6	C	600	ANP	PG-O2G	-2.28	1.50	1.56
6	D	600	ANP	PG-O3G	-2.26	1.50	1.56

The worst 5 of 114 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	M	600	ANP	N3-C2-N1	-7.78	122.93	128.89
6	J	600	ANP	N3-C2-N1	-7.72	122.98	128.89
6	X	600	ANP	N3-C2-N1	-7.57	123.10	128.89
6	A	600	ANP	N3-C2-N1	-7.36	123.25	128.89
6	U	600	ANP	N3-C2-N1	-7.32	123.29	128.89

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
6	T	600	ANP	O1B-PB-N3B-PG

There are no ring outliers.

10 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	600	ANP	2	0
6	C	600	ANP	3	0
6	D	600	ANP	2	0
6	F	600	ANP	3	0
6	J	600	ANP	3	0
6	K	600	ANP	1	0
6	M	600	ANP	3	0
6	T	600	ANP	2	0
6	V	600	ANP	2	0
6	X	600	ANP	2	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^{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	485/510 (95%)	-0.19	1 (0%) 95 94	49, 67, 102, 161	0
1	B	486/510 (95%)	0.08	13 (2%) 58 44	60, 94, 131, 172	0
1	C	484/510 (94%)	0.13	12 (2%) 61 47	62, 83, 134, 166	0
1	J	482/510 (94%)	0.18	20 (4%) 41 27	63, 91, 159, 179	0
1	K	483/510 (94%)	0.40	36 (7%) 17 9	78, 118, 163, 170	0
1	L	479/510 (93%)	0.15	17 (3%) 48 32	63, 88, 145, 168	0
1	S	483/510 (94%)	-0.04	7 (1%) 78 65	60, 84, 110, 171	0
1	T	484/510 (94%)	-0.03	4 (0%) 87 80	59, 84, 108, 143	0
1	U	485/510 (95%)	0.15	23 (4%) 35 22	81, 104, 132, 166	0
2	D	470/484 (97%)	0.04	9 (1%) 70 55	54, 80, 131, 155	0
2	E	469/484 (96%)	0.11	16 (3%) 49 34	56, 86, 126, 152	0
2	F	469/484 (96%)	0.11	9 (1%) 70 55	59, 89, 114, 134	0
2	M	460/484 (95%)	0.19	26 (5%) 27 15	63, 87, 146, 171	0
2	N	463/484 (95%)	0.46	46 (9%) 9 5	71, 115, 157, 166	0
2	O	469/484 (96%)	0.28	29 (6%) 24 13	78, 110, 159, 167	0
2	V	360/484 (74%)	0.43	27 (7%) 17 9	78, 109, 146, 178	0
2	W	468/484 (96%)	-0.14	4 (0%) 85 78	57, 72, 103, 143	0
2	X	469/484 (96%)	-0.03	4 (0%) 85 78	65, 91, 113, 132	0
3	G	268/278 (96%)	-0.01	1 (0%) 93 90	62, 92, 108, 115	0
3	P	268/278 (96%)	0.77	43 (16%) 3 2	82, 145, 165, 176	0
3	Y	115/278 (41%)	1.11	31 (26%) 1 0	73, 116, 148, 153	0
4	H	122/138 (88%)	0.00	0 100 100	76, 97, 150, 167	0
4	Q	101/138 (73%)	1.57	37 (36%) 0 0	138, 152, 169, 175	0
5	I	55/61 (90%)	0.03	1 (1%) 71 58	90, 111, 134, 149	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
5	R	55/61 (90%)	0.78	5 (9%) 11 6	126, 146, 163, 167	0
All	All	9432/10178 (92%)	0.17	421 (4%) 37 23	49, 93, 152, 179	0

The worst 5 of 421 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	M	396	LEU	9.5
4	Q	71	SER	7.1
2	V	144	LEU	5.9
4	Q	12	LEU	5.9
4	Q	54	PRO	5.8

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 carbohydrates 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. 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
7	MG	F	700	1/1	0.93	0.45	7.14	83,83,83,83	0
7	MG	M	700	1/1	0.96	0.43	6.74	80,80,80,80	0
7	MG	O	700	1/1	0.97	0.36	6.67	91,91,91,91	0
7	MG	X	700	1/1	0.98	0.43	5.94	80,80,80,80	0
7	MG	D	700	1/1	0.93	0.52	5.42	83,83,83,83	0
6	ANP	T	600	31/31	0.93	0.25	1.90	69,72,75,76	0
6	ANP	A	600	31/31	0.95	0.22	1.28	58,62,65,66	0
6	ANP	B	600	31/31	0.90	0.24	1.19	80,88,97,98	0
6	ANP	C	600	31/31	0.91	0.24	1.03	77,83,89,89	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
6	ANP	F	600	31/31	0.93	0.27	0.83	82,84,88,89	0
6	ANP	X	600	31/31	0.96	0.25	0.67	70,72,78,78	0
6	ANP	M	600	31/31	0.95	0.23	0.44	78,85,94,94	0
6	ANP	O	600	31/31	0.94	0.22	0.21	90,102,107,107	0
6	ANP	D	600	31/31	0.95	0.24	0.10	82,89,91,91	0
6	ANP	S	600	31/31	0.93	0.20	-0.08	83,85,86,86	0
6	ANP	J	600	31/31	0.93	0.20	-0.11	78,89,93,94	0
6	ANP	L	600	31/31	0.95	0.21	-0.17	83,86,87,88	0
6	ANP	U	600	31/31	0.95	0.20	-0.34	82,84,87,87	0
6	ANP	V	600	31/31	0.90	0.20	-0.55	114,116,117,118	0
6	ANP	K	600	31/31	0.88	0.18	-0.65	105,113,114,115	0
7	MG	B	700	1/1	0.93	0.48	-	82,82,82,82	0
7	MG	V	700	1/1	0.84	0.11	-	112,112,112,112	0
7	MG	A	700	1/1	0.95	0.44	-	66,66,66,66	0
7	MG	S	700	1/1	0.97	0.50	-	84,84,84,84	0
7	MG	T	700	1/1	0.96	0.64	-	76,76,76,76	0
7	MG	K	700	1/1	0.93	0.35	-	102,102,102,102	0
7	MG	U	700	1/1	0.95	0.46	-	83,83,83,83	0
7	MG	J	700	1/1	0.88	0.40	-	81,81,81,81	0
7	MG	L	700	1/1	0.93	0.40	-	86,86,86,86	0
7	MG	C	700	1/1	0.91	0.51	-	78,78,78,78	0

6.5 Other polymers (i)

There are no such residues in this entry.