



wwPDB X-ray Structure Validation Summary Report ⓘ

May 13, 2020 – 01:59 pm BST

PDB ID : 3FKS
Title : Yeast F1 ATPase in the absence of bound nucleotides
Authors : Kabaleeswaran, V.; Symersky, J.; Shen, H.; Walker, J.E.; Leslie, A.G.W.;
Mueller, D.M.
Deposited on : 2008-12-17
Resolution : 3.59 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

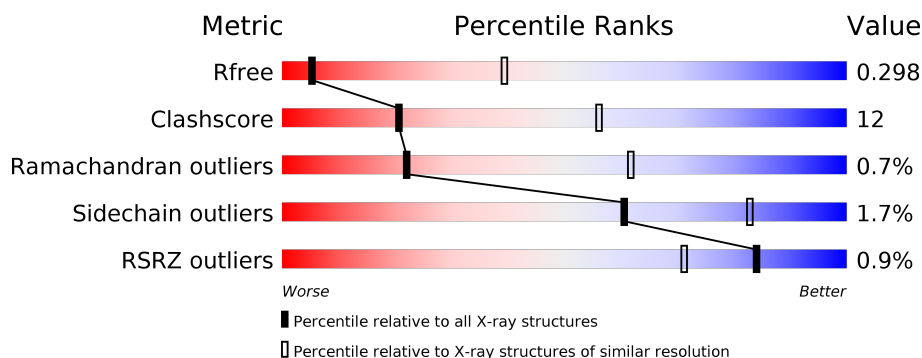
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 Å.

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





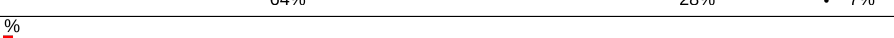


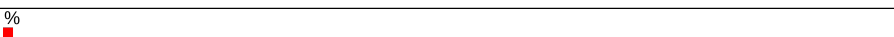
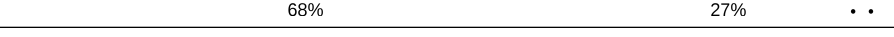


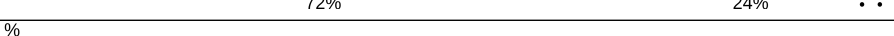


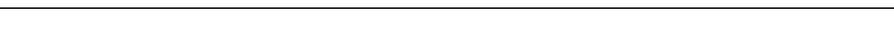
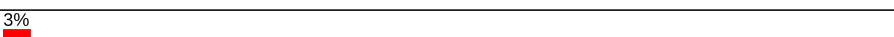
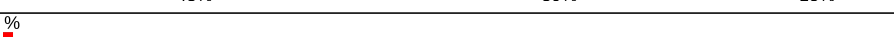
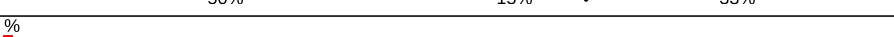





Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.66-3.50)
Clashscore	141614	1181 (3.66-3.50)
Ramachandran outliers	138981	1143 (3.66-3.50)
Sidechain outliers	138945	1143 (3.66-3.50)
RSRZ outliers	127900	1012 (3.66-3.50)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	510	
1	B	510	
1	C	510	
1	J	510	
1	K	510	
1	L	510	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 71793 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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	484	Total	C	N	O	S	0	0	0
			3679	2322	650	704	3			
1	B	479	Total	C	N	O	S	0	0	0
			3645	2302	645	695	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
			3656	2309	646	698	3			
1	K	484	Total	C	N	O	S	0	0	0
			3659	2309	650	697	3			
1	L	484	Total	C	N	O	S	0	0	0
			3680	2325	650	702	3			
1	S	481	Total	C	N	O	S	0	0	0
			3657	2310	646	698	3			
1	T	473	Total	C	N	O	S	0	0	0
			3596	2272	635	686	3			
1	U	477	Total	C	N	O	S	0	0	0
			3629	2296	643	687	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	466	Total	C	N	O	S	0	0	0
			3517	2232	599	680	6			
2	E	468	Total	C	N	O	S	0	0	0
			3536	2243	602	685	6			
2	F	471	Total	C	N	O	S	0	0	0
			3558	2255	606	691	6			
2	M	469	Total	C	N	O	S	0	0	0
			3540	2244	603	687	6			
2	N	466	Total	C	N	O	S	0	0	0
			3522	2235	600	681	6			

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	469	Total	C	N	O	S	0	0	0
			3539	2245	603	685	6			
2	V	455	Total	C	N	O	S	0	0	0
			3457	2192	589	670	6			
2	W	466	Total	C	N	O	S	0	0	0
			3526	2237	600	683	6			
2	X	469	Total	C	N	O	S	0	0	0
			3543	2247	603	687	6			

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
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

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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
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, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	268	Total	C	N	O	S	0	0	0
			2070	1300	357	403	10			
3	P	235	Total	C	N	O	S	0	0	0
			1766	1109	303	344	10			
3	Y	187	Total	C	N	O	S	0	0	0
			1444	901	257	277	9			

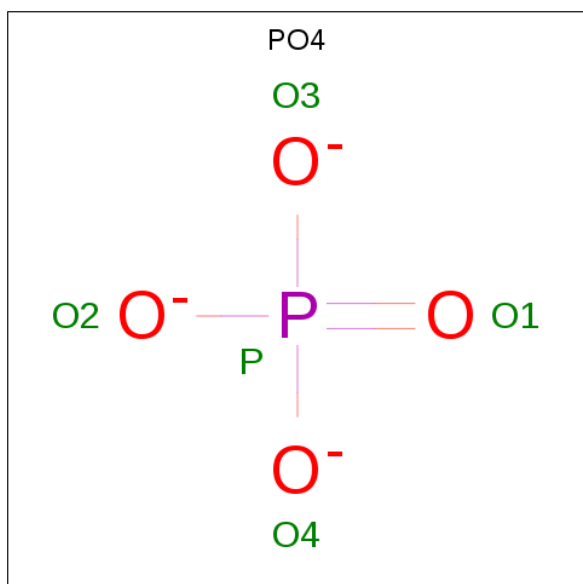
- Molecule 4 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	116	Total	C	N	O	S	0	0	0
			849	539	140	168	2			
4	Q	68	Total	C	N	O		0	0	0
			339	203	68	68				
4	Z	11	Total	C	N	O		0	0	0
			55	33	11	11				

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	46	Total	C	N	O	0	0	0
			326	209	51	66			
5	R	25	Total	C	N	O	0	0	0
			125	75	25	25			
5	1	25	Total	C	N	O	0	0	0
			125	75	25	25			

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).

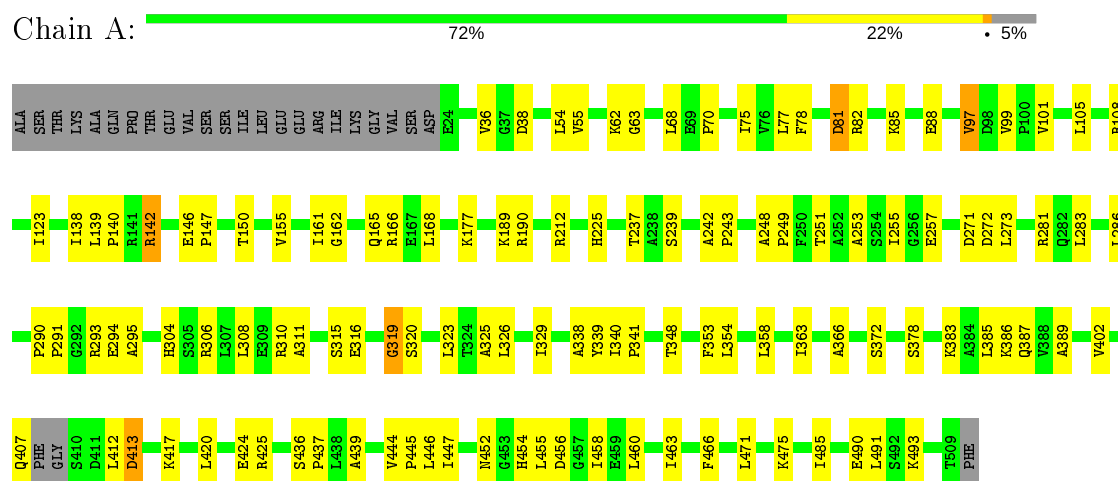


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	P	0	0
			5	4	1		
6	B	1	Total	O	P	0	0
			5	4	1		
6	C	1	Total	O	P	0	0
			5	4	1		
6	D	1	Total	O	P	0	0
			5	4	1		
6	F	1	Total	O	P	0	0
			5	4	1		
6	J	1	Total	O	P	0	0
			5	4	1		
6	K	1	Total	O	P	0	0
			5	4	1		
6	L	1	Total	O	P	0	0
			5	4	1		
6	M	1	Total	O	P	0	0
			5	4	1		
6	N	1	Total	O	P	0	0
			5	4	1		
6	O	1	Total	O	P	0	0
			5	4	1		
6	S	1	Total	O	P	0	0
			5	4	1		
6	T	1	Total	O	P	0	0
			5	4	1		
6	U	1	Total	O	P	0	0
			5	4	1		
6	X	1	Total	O	P	0	0
			5	4	1		

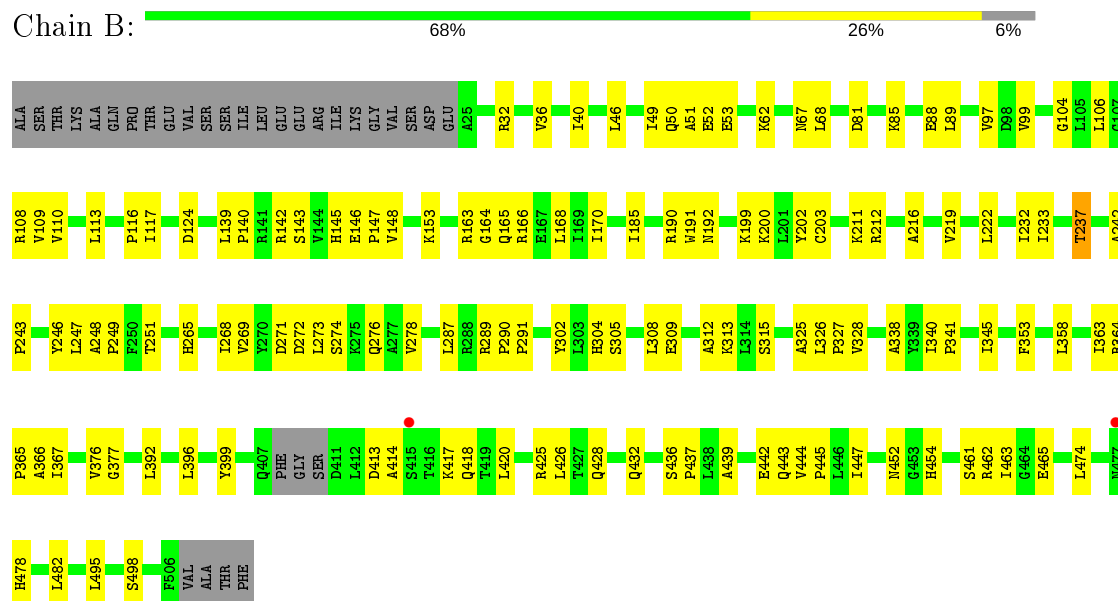
3 Residue-property plots

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

- Molecule 1: ATP synthase subunit alpha, mitochondrial

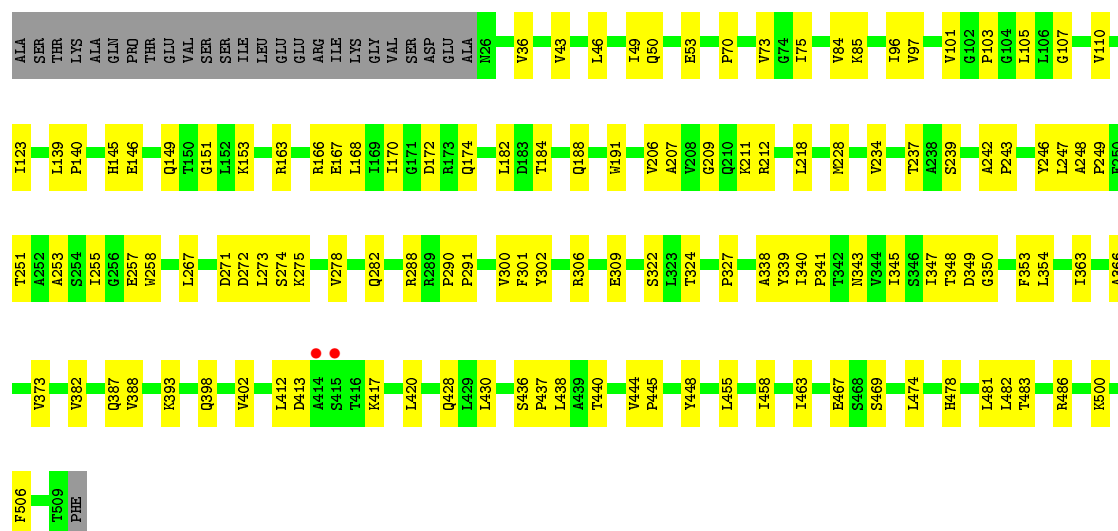


- Molecule 1: ATP synthase subunit alpha, mitochondrial



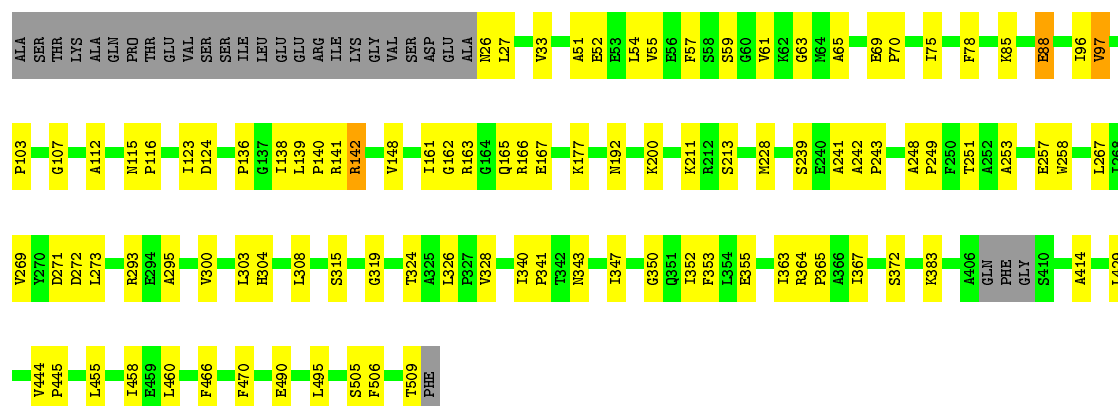
- Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain C:  71% 24% 5%



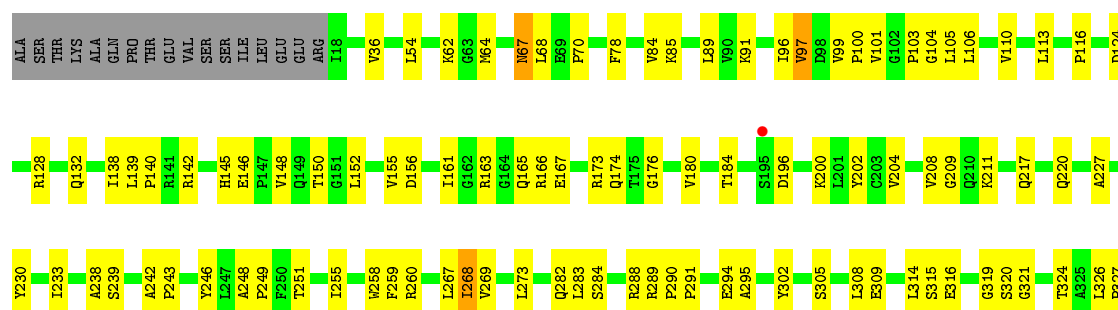
- Molecule 1: ATP synthase subunit alpha, mitochondrial

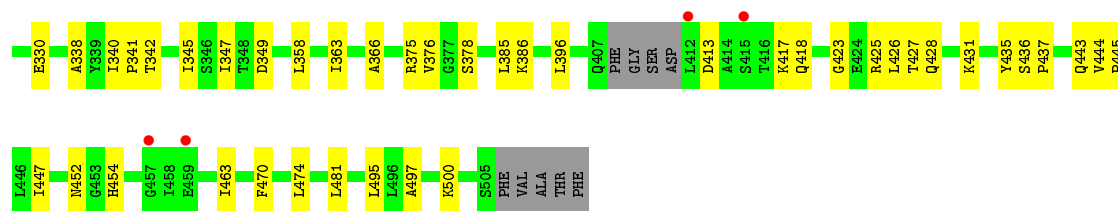
Chain J:  75% 19% 6%



- Molecule 1: ATP synthase subunit alpha, mitochondrial

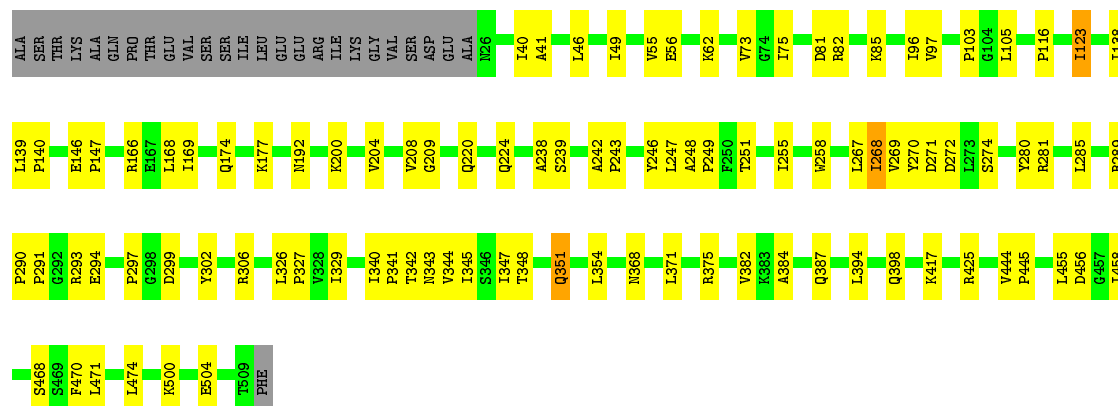
Chain K:  67% 27% 5%





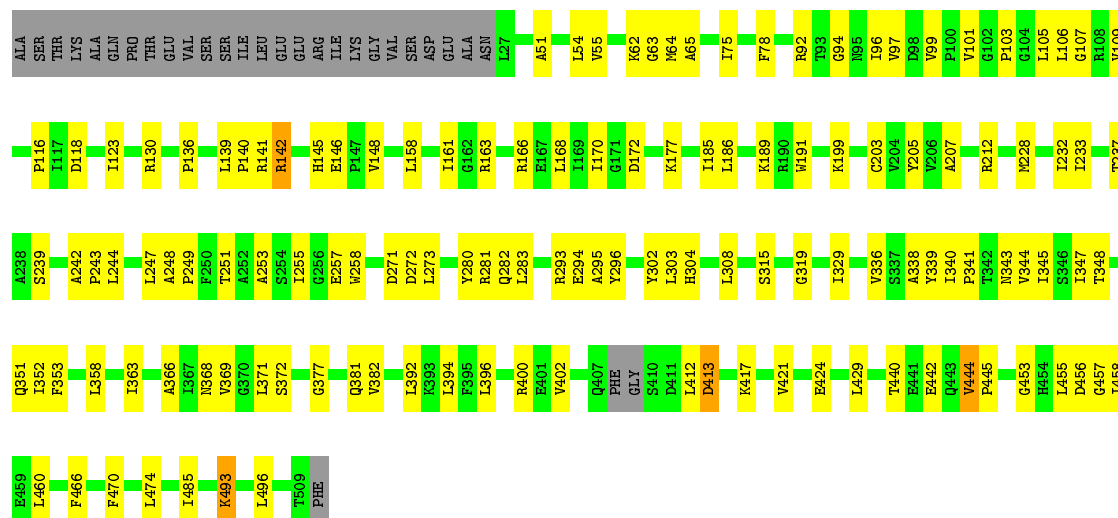
- Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain L: 75% 19% • 5%



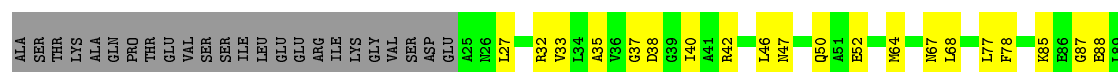
- Molecule 1: ATP synthase subunit alpha, mitochondrial

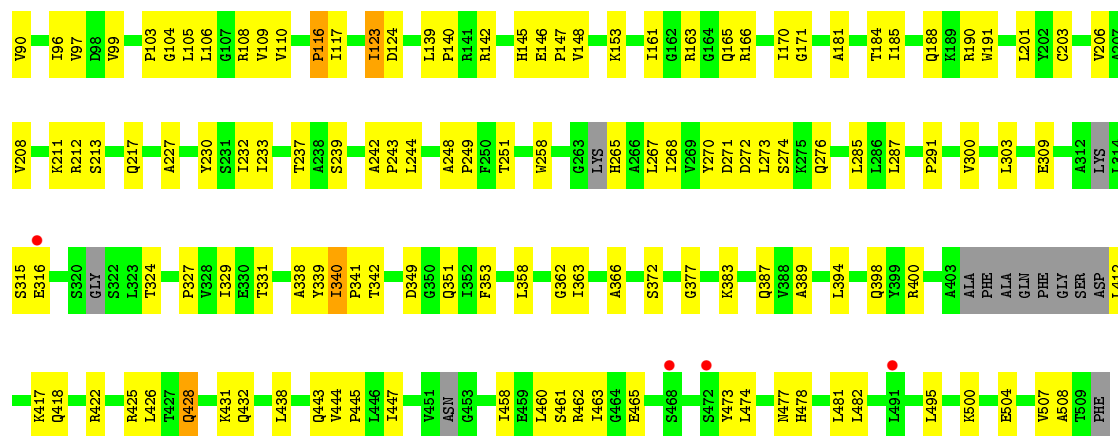
Chain S: 68% 25% • 6%



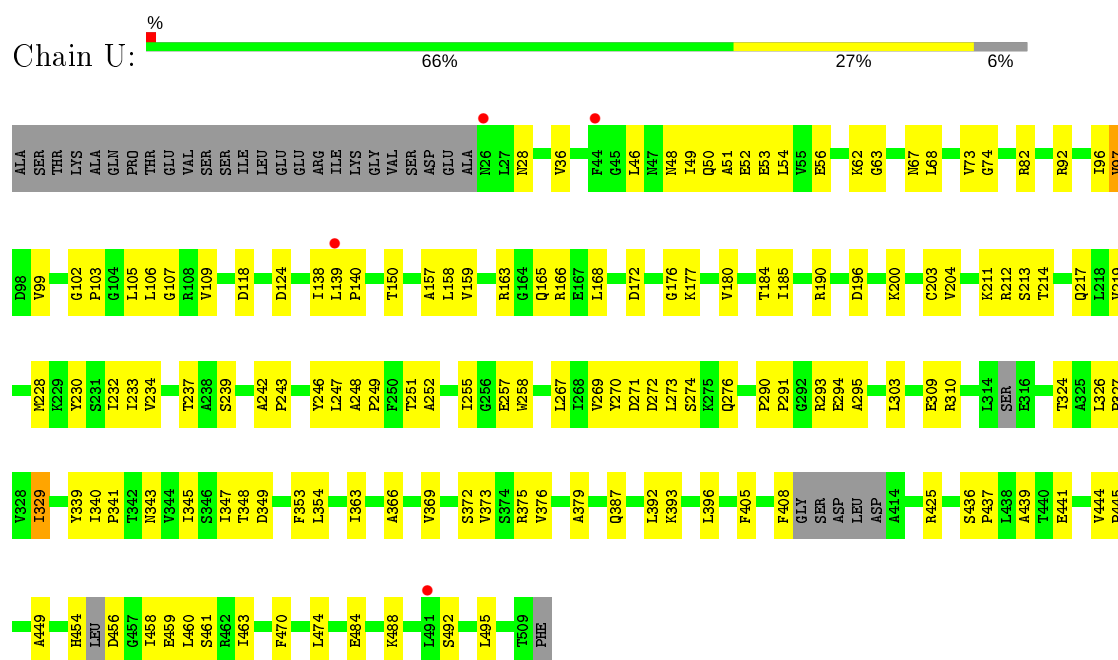
- Molecule 1: ATP synthase subunit alpha, mitochondrial

Chain T: 64% 28% • 7%

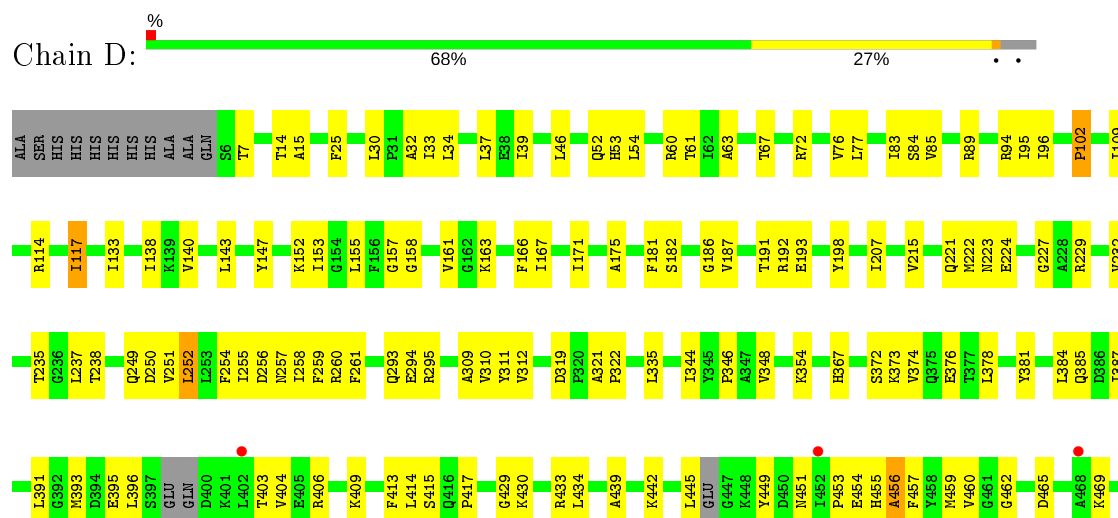


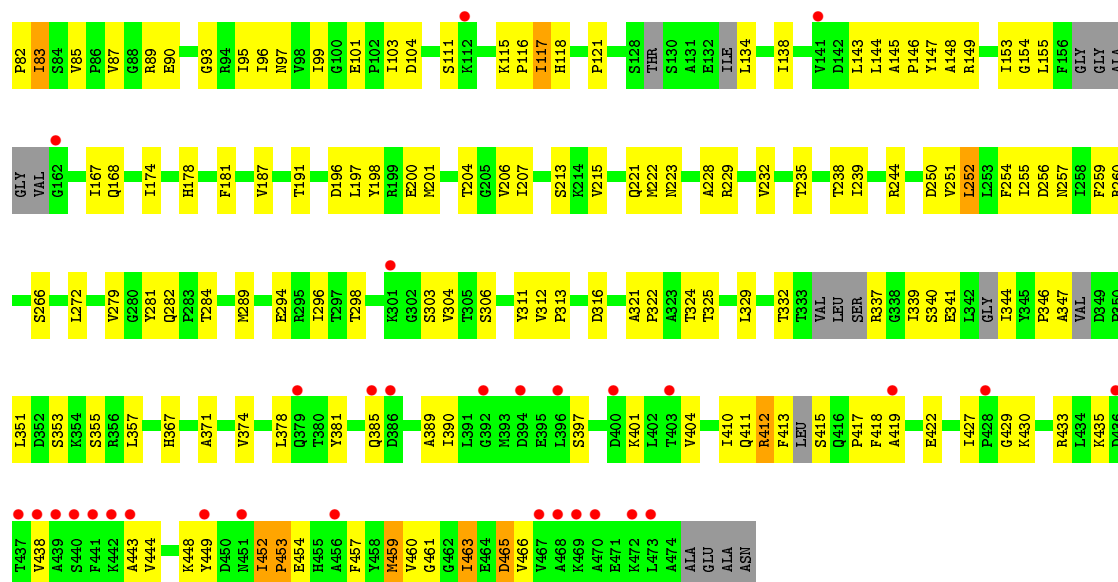


• Molecule 1: ATP synthase subunit alpha, mitochondrial



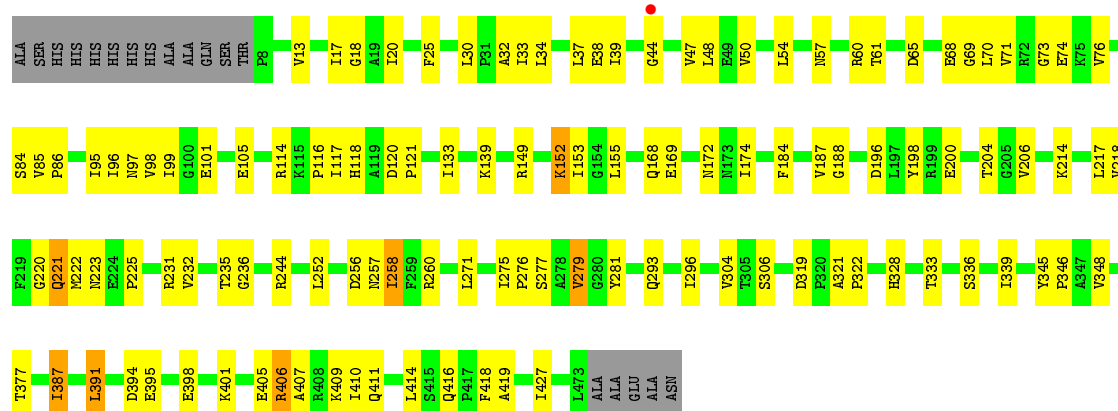
• Molecule 2: ATP synthase subunit beta, mitochondrial





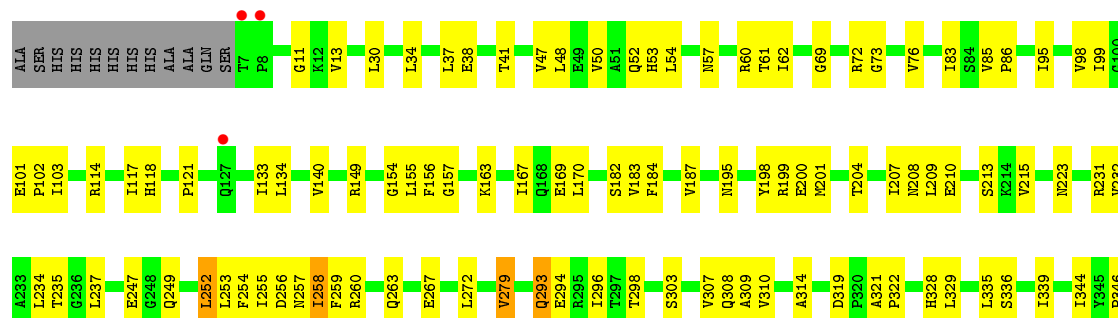
• Molecule 2: ATP synthase subunit beta, mitochondrial

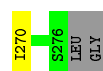
Chain W: 72% 23%



• Molecule 2: ATP synthase subunit beta, mitochondrial

Chain X: 71% 25%

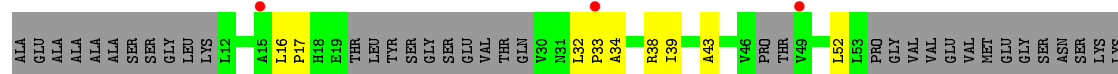
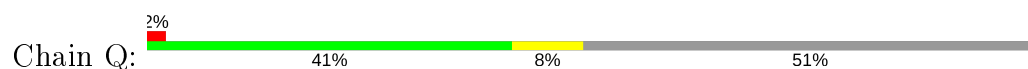




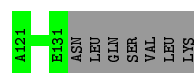
- Molecule 4: ATP synthase subunit delta, mitochondrial



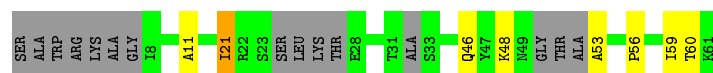
- Molecule 4: ATP synthase subunit delta, mitochondrial



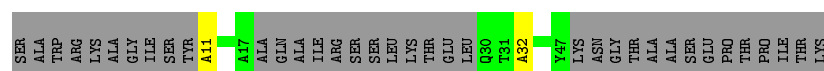
- Molecule 4: ATP synthase subunit delta, mitochondrial



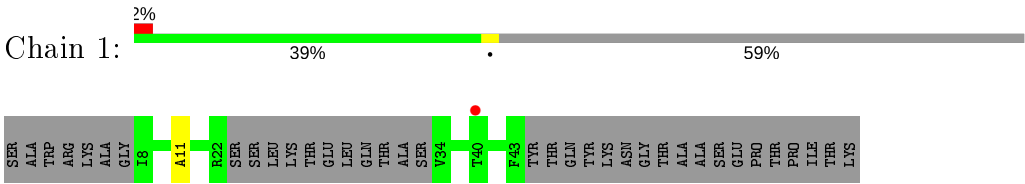
- Molecule 5: ATP synthase subunit epsilon, mitochondrial



- Molecule 5: ATP synthase subunit epsilon, mitochondrial



● Molecule 5: ATP synthase subunit epsilon, mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	111.93Å 290.49Å 188.70Å 90.00° 101.75° 90.00°	Depositor
Resolution (Å)	33.20 – 3.59 33.20 – 3.59	Depositor EDS
% Data completeness (in resolution range)	98.1 (33.20-3.59) 98.1 (33.20-3.59)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 3.56Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.242 , 0.306 0.231 , 0.298	Depositor DCC
R_{free} test set	2727 reflections (2.02%)	wwPDB-VP
Wilson B-factor (Å ²)	111.7	Xtriage
Anisotropy	0.115	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 50.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	71793	wwPDB-VP
Average B, all atoms (Å ²)	113.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.48% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4

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	0.20	0/3733	0.36	0/5052
1	B	0.20	0/3699	0.36	0/5005
1	C	0.20	0/3736	0.36	0/5057
1	J	0.20	0/3710	0.36	0/5021
1	K	0.20	0/3712	0.36	0/5023
1	L	0.20	0/3736	0.36	0/5057
1	S	0.23	0/3711	0.37	0/5022
1	T	0.20	0/3645	0.36	0/4929
1	U	0.20	0/3682	0.36	0/4979
2	D	0.22	0/3571	0.39	0/4840
2	E	0.21	0/3592	0.38	0/4870
2	F	0.20	0/3614	0.39	0/4901
2	M	0.22	0/3596	0.39	0/4877
2	N	0.20	0/3577	0.38	0/4848
2	O	0.20	0/3595	0.39	0/4876
2	V	0.21	0/3506	0.39	0/4742
2	W	0.20	0/3582	0.38	0/4856
2	X	0.20	0/3599	0.39	0/4881
3	G	0.22	0/2096	0.37	0/2822
3	P	0.24	0/1780	0.42	0/2388
3	Y	0.21	0/1451	0.37	0/1939
4	H	0.21	0/858	0.36	0/1161
4	Q	0.26	0/334	0.42	0/457
4	Z	0.16	0/54	0.36	0/74
5	1	0.34	0/123	0.43	0/169
5	I	0.20	0/329	0.38	0/449
5	R	0.18	0/123	0.33	0/169
All	All	0.21	0/72744	0.38	0/98464

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

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	3679	0	3762	80	0
1	B	3645	0	3730	90	0
1	C	3680	0	3764	92	0
1	J	3656	0	3743	66	0
1	K	3659	0	3732	98	0
1	L	3680	0	3764	79	0
1	S	3657	0	3745	102	0
1	T	3596	0	3681	108	0
1	U	3629	0	3710	90	0
2	D	3517	0	3594	106	0
2	E	3536	0	3610	96	0
2	F	3558	0	3629	104	0
2	M	3540	0	3607	77	0
2	N	3522	0	3598	101	0
2	O	3539	0	3612	89	0
2	V	3457	0	3510	120	0
2	W	3526	0	3600	83	0
2	X	3543	0	3616	84	0
3	G	2070	0	2128	49	0
3	P	1766	0	1794	89	0
3	Y	1444	0	1491	31	0
4	H	849	0	845	35	0
4	Q	339	0	160	4	0
4	Z	55	0	30	0	0
5	1	125	0	66	0	0
5	I	326	0	286	7	0
5	R	125	0	63	1	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
6	C	5	0	0	0	0
6	D	5	0	0	0	0
6	F	5	0	0	0	0
6	J	5	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	K	5	0	0	0	0
6	L	5	0	0	0	0
6	M	5	0	0	0	0
6	N	5	0	0	0	0
6	O	5	0	0	0	0
6	S	5	0	0	0	0
6	T	5	0	0	0	0
6	U	5	0	0	0	0
6	X	5	0	0	0	0
All	All	71793	0	72870	1775	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 12.

The worst 5 of 1775 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:S:444:VAL:HG23	1:S:445:PRO:HD3	1.47	0.96
1:A:85:LYS:HE2	2:D:32:ALA:HB2	1.47	0.96
1:U:73:VAL:HG22	2:V:72:ARG:HH22	1.33	0.93
4:H:102:LYS:HG2	4:H:105:LEU:HD11	1.49	0.93
2:M:237:LEU:HD11	2:M:296:ILE:HG12	1.53	0.90

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	480/510 (94%)	437 (91%)	40 (8%)	3 (1%)	25	64
1	B	475/510 (93%)	430 (90%)	41 (9%)	4 (1%)	19	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	482/510 (94%)	449 (93%)	32 (7%)	1 (0%)	47	80
1	J	477/510 (94%)	447 (94%)	27 (6%)	3 (1%)	25	64
1	K	480/510 (94%)	442 (92%)	35 (7%)	3 (1%)	25	64
1	L	482/510 (94%)	453 (94%)	29 (6%)	0	100	100
1	S	477/510 (94%)	440 (92%)	32 (7%)	5 (1%)	15	55
1	T	461/510 (90%)	414 (90%)	43 (9%)	4 (1%)	17	57
1	U	469/510 (92%)	427 (91%)	41 (9%)	1 (0%)	47	80
2	D	460/484 (95%)	417 (91%)	40 (9%)	3 (1%)	22	62
2	E	466/484 (96%)	422 (91%)	41 (9%)	3 (1%)	25	64
2	F	469/484 (97%)	436 (93%)	32 (7%)	1 (0%)	47	80
2	M	467/484 (96%)	430 (92%)	35 (8%)	2 (0%)	34	71
2	N	462/484 (96%)	429 (93%)	30 (6%)	3 (1%)	25	64
2	O	467/484 (96%)	434 (93%)	32 (7%)	1 (0%)	47	80
2	V	439/484 (91%)	381 (87%)	55 (12%)	3 (1%)	22	62
2	W	464/484 (96%)	414 (89%)	43 (9%)	7 (2%)	10	47
2	X	467/484 (96%)	435 (93%)	31 (7%)	1 (0%)	47	80
3	G	264/278 (95%)	244 (92%)	19 (7%)	1 (0%)	34	71
3	P	221/278 (80%)	200 (90%)	17 (8%)	4 (2%)	8	43
3	Y	169/278 (61%)	153 (90%)	14 (8%)	2 (1%)	13	51
4	H	108/138 (78%)	92 (85%)	16 (15%)	0	100	100
4	Q	56/138 (41%)	40 (71%)	12 (21%)	4 (7%)	1	14
4	Z	9/138 (6%)	5 (56%)	4 (44%)	0	100	100
5	I	21/61 (34%)	14 (67%)	6 (29%)	1 (5%)	2	22
5	I	38/61 (62%)	34 (90%)	3 (8%)	1 (3%)	5	35
5	R	21/61 (34%)	15 (71%)	5 (24%)	1 (5%)	2	22
All	All	9351/10377 (90%)	8534 (91%)	755 (8%)	62 (1%)	22	62

5 of 62 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	413	ASP
2	D	456	ALA
3	P	192	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	Q	17	PRO
4	Q	39	ILE

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	390/412 (95%)	386 (99%)	4 (1%)	76	89
1	B	386/412 (94%)	381 (99%)	5 (1%)	69	87
1	C	390/412 (95%)	387 (99%)	3 (1%)	81	92
1	J	388/412 (94%)	383 (99%)	5 (1%)	69	87
1	K	384/412 (93%)	376 (98%)	8 (2%)	53	79
1	L	390/412 (95%)	384 (98%)	6 (2%)	65	85
1	S	388/412 (94%)	384 (99%)	4 (1%)	76	89
1	T	382/412 (93%)	375 (98%)	7 (2%)	59	81
1	U	382/412 (93%)	376 (98%)	6 (2%)	62	83
2	D	377/390 (97%)	368 (98%)	9 (2%)	49	76
2	E	378/390 (97%)	374 (99%)	4 (1%)	73	88
2	F	381/390 (98%)	374 (98%)	7 (2%)	59	81
2	M	378/390 (97%)	372 (98%)	6 (2%)	62	83
2	N	377/390 (97%)	368 (98%)	9 (2%)	49	76
2	O	378/390 (97%)	374 (99%)	4 (1%)	73	88
2	V	370/390 (95%)	359 (97%)	11 (3%)	41	72
2	W	378/390 (97%)	372 (98%)	6 (2%)	62	83
2	X	379/390 (97%)	375 (99%)	4 (1%)	73	88
3	G	228/236 (97%)	225 (99%)	3 (1%)	69	87
3	P	188/236 (80%)	179 (95%)	9 (5%)	25	60
3	Y	157/236 (66%)	153 (98%)	4 (2%)	47	75
4	H	92/112 (82%)	87 (95%)	5 (5%)	22	57

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	Q	1/112 (1%)	1 (100%)	0	100	100
5	I	29/48 (60%)	29 (100%)	0	100	100
All	All	7571/8198 (92%)	7442 (98%)	129 (2%)	60	83

5 of 129 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	456	ASP
2	N	406	ARG
2	W	394	ASP
2	M	117	ILE
2	N	17	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 86 such sidechains are listed below:

Mol	Chain	Res	Type
1	K	210	GLN
2	N	27	GLN
2	X	365	GLN
1	K	454	HIS
1	L	225	HIS

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](#)

15 ligands are modelled in this entry.

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	PO4	F	605	-	4,4,4	0.99	0	6,6,6	0.42	0
6	PO4	O	611	-	4,4,4	0.94	0	6,6,6	0.39	0
6	PO4	B	602	-	4,4,4	0.93	0	6,6,6	0.41	0
6	PO4	L	608	-	4,4,4	0.99	0	6,6,6	0.43	0
6	PO4	T	613	-	4,4,4	0.91	0	6,6,6	0.43	0
6	PO4	A	601	-	4,4,4	0.92	0	6,6,6	0.41	0
6	PO4	U	614	-	4,4,4	0.96	0	6,6,6	0.46	0
6	PO4	K	607	-	4,4,4	0.99	0	6,6,6	0.42	0
6	PO4	X	615	-	4,4,4	0.93	0	6,6,6	0.47	0
6	PO4	D	604	-	4,4,4	0.86	0	6,6,6	0.46	0
6	PO4	M	609	-	4,4,4	0.93	0	6,6,6	0.46	0
6	PO4	J	606	-	4,4,4	0.94	0	6,6,6	0.44	0
6	PO4	N	610	-	4,4,4	0.92	0	6,6,6	0.42	0
6	PO4	C	603	-	4,4,4	0.95	0	6,6,6	0.45	0
6	PO4	S	612	-	4,4,4	0.93	0	6,6,6	0.46	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	484/510 (94%)	-0.42	0 100 100	70, 104, 128, 143	0
1	B	479/510 (93%)	-0.27	2 (0%) 92 86	73, 113, 139, 148	0
1	C	484/510 (94%)	-0.39	2 (0%) 92 86	78, 108, 133, 145	0
1	J	481/510 (94%)	-0.34	0 100 100	83, 111, 134, 143	0
1	K	484/510 (94%)	-0.27	5 (1%) 82 69	76, 112, 139, 147	0
1	L	484/510 (94%)	-0.39	0 100 100	70, 94, 126, 144	0
1	S	481/510 (94%)	-0.34	0 100 100	81, 112, 130, 141	0
1	T	473/510 (92%)	-0.19	4 (0%) 86 73	99, 123, 140, 147	0
1	U	477/510 (93%)	-0.09	4 (0%) 86 73	102, 123, 134, 141	0
2	D	466/484 (96%)	-0.20	3 (0%) 89 80	85, 116, 138, 145	0
2	E	468/484 (96%)	-0.29	3 (0%) 89 80	68, 111, 136, 149	0
2	F	471/484 (97%)	-0.39	1 (0%) 95 91	73, 109, 128, 144	0
2	M	469/484 (96%)	-0.36	2 (0%) 92 86	80, 105, 128, 149	0
2	N	466/484 (96%)	-0.29	3 (0%) 89 80	71, 113, 132, 143	0
2	O	469/484 (96%)	-0.43	0 100 100	70, 106, 125, 134	0
2	V	455/484 (94%)	0.25	33 (7%) 15 8	99, 129, 146, 154	0
2	W	466/484 (96%)	-0.32	1 (0%) 95 91	89, 113, 129, 142	0
2	X	469/484 (96%)	-0.30	3 (0%) 89 80	93, 118, 135, 147	0
3	G	268/278 (96%)	-0.24	1 (0%) 92 86	72, 110, 128, 138	0
3	P	235/278 (84%)	0.04	9 (3%) 40 25	65, 127, 143, 150	0
3	Y	187/278 (67%)	-0.03	2 (1%) 80 66	96, 125, 139, 146	0
4	H	116/138 (84%)	-0.06	2 (1%) 70 53	93, 114, 137, 146	0
4	Q	68/138 (49%)	0.60	3 (4%) 34 20	98, 127, 135, 142	0
4	Z	11/138 (7%)	-0.12	0 100 100	129, 134, 140, 142	0

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
5	1	25/61 (40%)	0.27	1 (4%) 38 23	112, 131, 137, 138	0
5	I	46/61 (75%)	-0.33	0 100 100	101, 115, 125, 130	0
5	R	25/61 (40%)	-0.15	0 100 100	118, 131, 139, 144	0
All	All	9507/10377 (91%)	-0.26	84 (0%) 84 71	65, 114, 137, 154	0

The worst 5 of 84 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	V	440	SER	7.4
2	V	437	THR	5.3
2	V	392	GLY	4.9
2	V	441	PHE	4.6
2	V	469	LYS	3.8

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	PO4	D	604	5/5	0.88	0.22	134,136,139,154	0
6	PO4	S	612	5/5	0.88	0.27	106,107,112,116	0
6	PO4	U	614	5/5	0.92	0.24	96,96,100,113	0
6	PO4	A	601	5/5	0.92	0.26	89,90,97,113	0
6	PO4	T	613	5/5	0.93	0.15	101,105,109,116	0
6	PO4	B	602	5/5	0.93	0.18	95,103,112,112	0
6	PO4	N	610	5/5	0.94	0.25	89,100,104,116	0
6	PO4	O	611	5/5	0.94	0.25	94,96,102,107	0
6	PO4	J	606	5/5	0.94	0.29	90,91,94,97	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	PO4	X	615	5/5	0.95	0.33	107,125,125,126	0
6	PO4	L	608	5/5	0.95	0.13	82,82,87,96	0
6	PO4	C	603	5/5	0.96	0.21	86,89,99,99	0
6	PO4	F	605	5/5	0.96	0.18	92,93,98,101	0
6	PO4	M	609	5/5	0.97	0.18	92,97,106,108	0
6	PO4	K	607	5/5	0.97	0.12	85,94,97,101	0

6.5 Other polymers [i](#)

There are no such residues in this entry.