W O R L D W I D E

wwPDB

P R O T E I N D A T A B A N K

wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 08:11 PM GMT

PDB ID   :   4XD7
Title   :   Structure of thermophilic F1-ATPase inhibited by epsilon subunit
Authors   :   SHIRAKIHARA, Y.; SHIRATORI, A.; TANIKAWA, H.; NAKASAKO, M.;
                YOSHIDA, M.; SUZUK, T.
Deposited on :   2014-12-19
Resolution :   3.90 Å(reported)

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

|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
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)	:	rb-20026982

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 3.90 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.
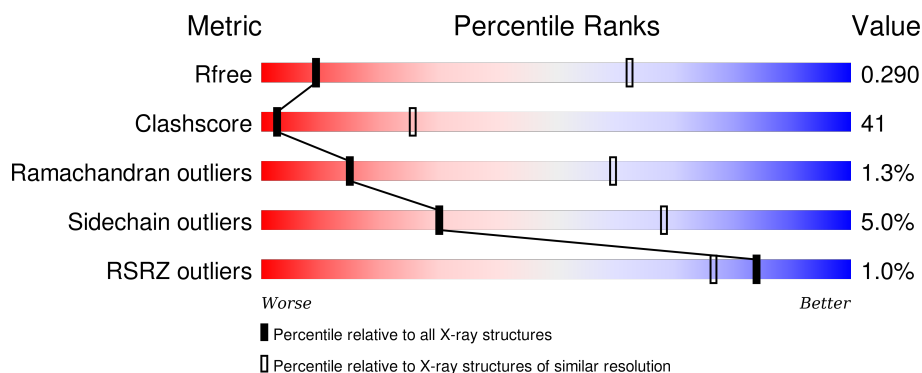
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	1014 (4.28-3.52)
Clashscore	102246	1031 (4.24-3.56)
Ramachandran outliers	100387	1012 (4.26-3.54)
Sidechain outliers	100360	1004 (4.26-3.54)
RSRZ outliers	91569	1018 (4.28-3.52)

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	502	37% 55% • 5%
1	B	502	2% 42% 40% • 16%
1	C	502	43% 48% • 5%
2	D	483	48% 47% • •
2	E	483	43% 51% • •

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Mol	Chain	Length	Quality of chain
2	F	483	% 53% 42% • •
3	G	285	39% 44% 6% 11%
4	H	133	4% 45% 46% 6% •

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
5	SO4	A	700	-	-	X	X
5	SO4	E	700	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 22656 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	477	Total 3462	C 2189	N 606	O 658	Se 9	0	0	0
1	B	423	Total 2833	C 1786	N 484	O 554	Se 9	0	0	0
1	C	475	Total 3329	C 2109	N 577	O 634	Se 9	1	0	0

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	193	SER	CYS	conflict	UNP Q5KUJ1
A	254	LYS	GLN	conflict	UNP Q5KUJ1
A	463	PHE	TRP	conflict	UNP Q5KUJ1
B	193	SER	CYS	conflict	UNP Q5KUJ1
B	254	LYS	GLN	conflict	UNP Q5KUJ1
B	463	PHE	TRP	conflict	UNP Q5KUJ1
C	193	SER	CYS	conflict	UNP Q5KUJ1
C	254	LYS	GLN	conflict	UNP Q5KUJ1
C	463	PHE	TRP	conflict	UNP Q5KUJ1

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	470	Total 3480	C 2199	N 599	O 669	Se 13	1	0	0
2	E	469	Total 3484	C 2198	N 598	O 676	Se 12	0	0	0
2	F	464	Total 3334	C 2097	N 580	O 644	Se 13	4	0	0

There are 33 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	MSE	-	initiating methionine	UNP Q5KUJ3
D	-8	HIS	-	expression tag	UNP Q5KUJ3
D	-7	HIS	-	expression tag	UNP Q5KUJ3
D	-6	HIS	-	expression tag	UNP Q5KUJ3
D	-5	HIS	-	expression tag	UNP Q5KUJ3
D	-4	HIS	-	expression tag	UNP Q5KUJ3
D	-3	HIS	-	expression tag	UNP Q5KUJ3
D	-2	HIS	-	expression tag	UNP Q5KUJ3
D	-1	HIS	-	expression tag	UNP Q5KUJ3
D	0	HIS	-	expression tag	UNP Q5KUJ3
D	1	HIS	-	expression tag	UNP Q5KUJ3
E	-9	MSE	-	initiating methionine	UNP Q5KUJ3
E	-8	HIS	-	expression tag	UNP Q5KUJ3
E	-7	HIS	-	expression tag	UNP Q5KUJ3
E	-6	HIS	-	expression tag	UNP Q5KUJ3
E	-5	HIS	-	expression tag	UNP Q5KUJ3
E	-4	HIS	-	expression tag	UNP Q5KUJ3
E	-3	HIS	-	expression tag	UNP Q5KUJ3
E	-2	HIS	-	expression tag	UNP Q5KUJ3
E	-1	HIS	-	expression tag	UNP Q5KUJ3
E	0	HIS	-	expression tag	UNP Q5KUJ3
E	1	HIS	-	expression tag	UNP Q5KUJ3
F	-9	MSE	-	initiating methionine	UNP Q5KUJ3
F	-8	HIS	-	expression tag	UNP Q5KUJ3
F	-7	HIS	-	expression tag	UNP Q5KUJ3
F	-6	HIS	-	expression tag	UNP Q5KUJ3
F	-5	HIS	-	expression tag	UNP Q5KUJ3
F	-4	HIS	-	expression tag	UNP Q5KUJ3
F	-3	HIS	-	expression tag	UNP Q5KUJ3
F	-2	HIS	-	expression tag	UNP Q5KUJ3
F	-1	HIS	-	expression tag	UNP Q5KUJ3
F	0	HIS	-	expression tag	UNP Q5KUJ3
F	1	HIS	-	expression tag	UNP Q5KUJ3

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
3	G	254	1797	1142	308	339	1	7	0	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	109	CYS	SER	conflict	UNP Q5KUJ2

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	129	Total 890	C 563	N 148	O 175	Se 4	0	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).
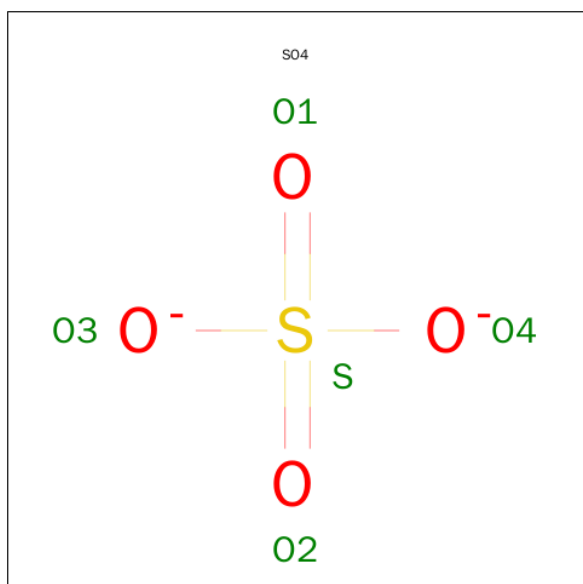
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 5	O S 4 1	0	0
5	B	1	Total 5	O S 4 1	0	0
5	D	1	Total 5	O S 4 1	0	0
5	E	1	Total 5	O S 4 1	0	0

- Molecule 6 is A D E N O S I N E - 5'- D I P H O S P H A T E (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
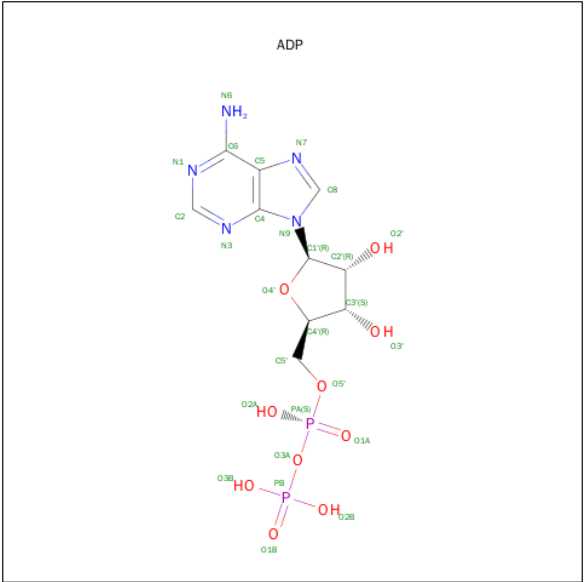
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
6	F	1	27	10	5	10	2	0	0

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

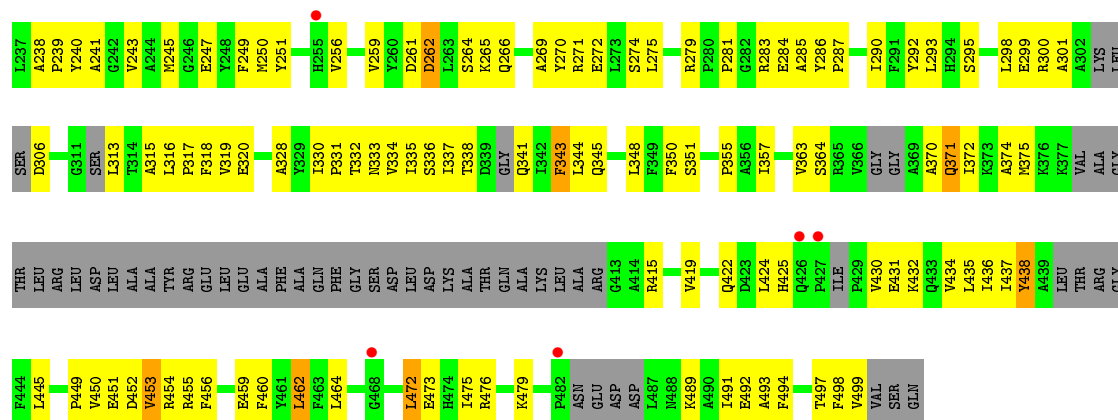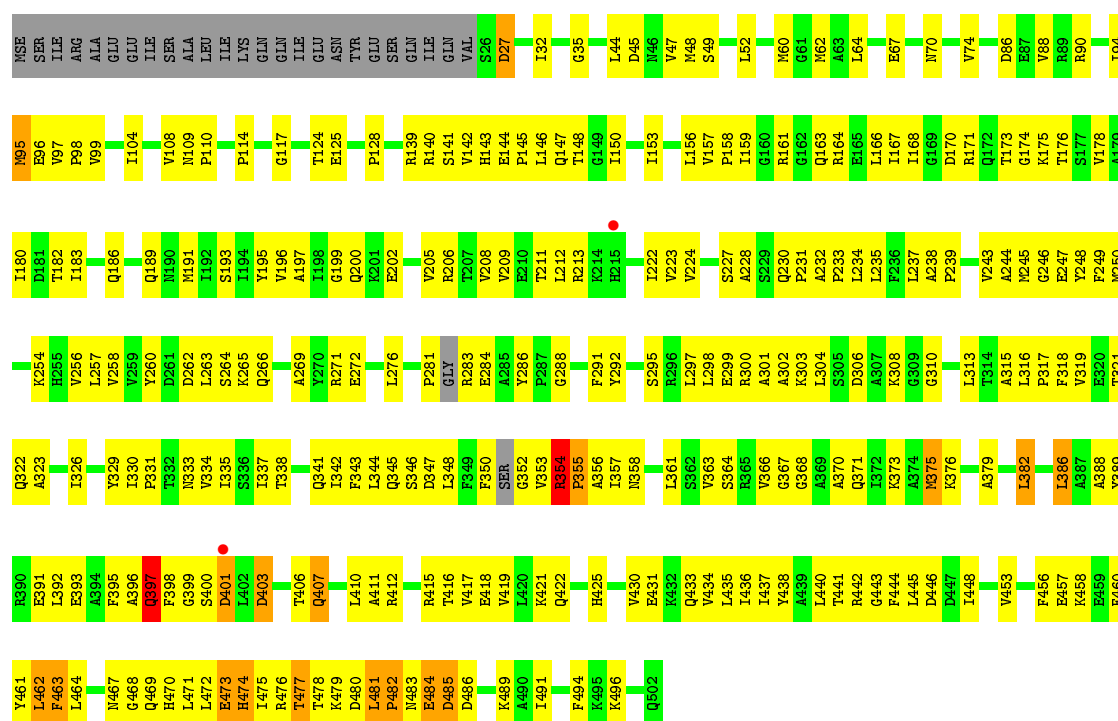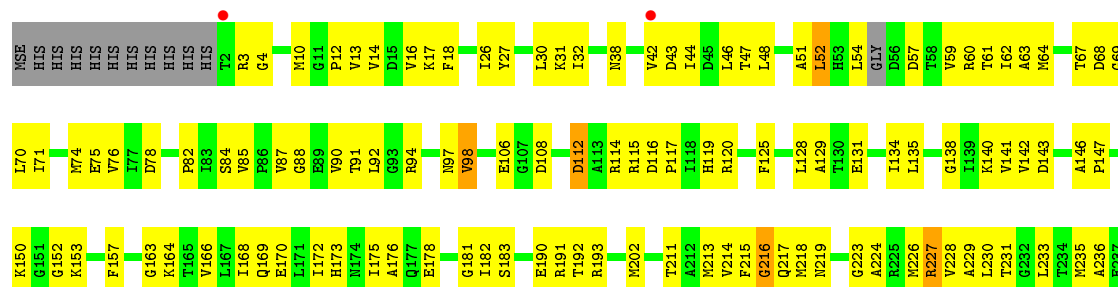L237 A238 P239 Y240 A241 G242 V243 A244 M245 G246 E247 Y248 F249 M250 Y251 H255 V256 V259 Y260 V259 D261 D262 L263 S264 K265 Q266 A269 Y270 R271 E272 L273 S274 L275 R279 R280 P281 G282 R283 E284 A285 Y286 P287 I290 Y291 Y292 L293 H294 S295 L298 E299 R300 A301 A302 LYS LEU

SER D306 G311 SER L313 T314 A315 L316 P317 F318 V319 E320 A328 Y329 I330 P331 T332 N333 V334 I335 S336 I337 T338 D339 GLY Q341 I342 F343 L344 Q345 L348 F349 S351 P355 A356 I357 V363 S364 R365 V366 GLY GLY A369 A370 Q371 I372 K373 A374 M375 K376 K377 VAL ALA GLY

THR LEU ARG LEU ASP LEU ALA ALA TYR ARG GLU LEU GLU ALA PHE ALA GLN PHE GLY ASP SER ASP LEU ASP LYS ALA THR GLN ALA LYS LEU ALA ARG G413 A414 R415 V419 Q422 D423 L424 H425 Q426 P427 ILE P429 V430 E431 K432 V434 L435 I436 I437 Y438 A439 LEU THR ARG GLY

F444 L445 P449 V450 F451 D452 V453 R454 R455 F456 E459 F460 Y461 L462 F463 L464 G468 L472 E473 H474 I475 R476 K479 P482 ASN GLU ASP L487 N488 K489 A490 I491 E492 A493 E494 T497 F498 V499 VAL SER GLN

• Molecule 1: ATP synthase subunit alpha

Chain C: 43% 48% • 5%

MSE SER ILE ARG ALA GLU GLU ILE SER ALA LEU ILE LYS GLN ILE GLU ASN TYR GLU SER GLN ILE GLN VAL S26 D27 I32 G35 L44 D45 N46 V47 M48 S49 L52 M60 G61 M62 A63 L64 E67 N70 V74 D86 E87 V88 R89 R90 I94

M95 E96 V97 P98 V99 I104 V108 M109 P110 P114 G117 T124 E125 P128 R139 R140 S141 V142 H143 E144 L146 Q147 T148 G149 I150 I153 L156 V157 P158 I159 G160 R161 G162 Q163 R164 E165 L166 I167 I168 G169 D170 R171 Q172 T173 G174 K175 T176 S177 V178 A179

I180 D181 T182 I183 Q186 Q189 M190 M191 I192 S193 I194 Y195 V196 A197 I198 G199 Q200 K201 E202 V205 R206 T207 V208 V209 E210 T211 L212 R213 K214 H215 I222 V223 V224 S227 A228 S229 Q230 P231 A232 P233 L234 L235 F236 L237 A238 P239 V243 A244 M245 G246 E247 Y248 F249 M250

K254 H255 V256 L257 V258 V259 Y260 D261 D262 L263 S264 K265 Q266 A269 Y270 R271 E272 L276 P281 GLY R283 E284 A285 Y286 P287 G288 F291 Y292 S295 R296 L297 L298 E299 R300 A301 A302 K303 L304 S305 D306 A307 K308 G309 G310 L313 T314 A315 L316 P317 F318 V319 E320 T321

Q322 A323 I326 Y329 I330 P331 T332 N333 V334 I335 S336 I337 T338 Q341 I342 F343 L344 Q345 S346 D347 L348 F349 F350 SER G352 V353 R354 P355 A356 I357 N358 L361 S362 V363 S364 R365 V366 G367 G368 A369 A370 Q371 I372 K373 A374 M375 K376 A379 L382 L386 A387 A388 Y389

R390 E391 L392 E393 A394 F395 A396 Q397 F398 G399 S400 D401 L402 D403 T406 Q407 L410 A411 R412 R415 T416 V417 E418 V419 L420 K421 Q422 H425 V430 E431 K432 Q433 V434 L435 I436 I437 Y438 A439 L440 T441 R442 G443 F444 L445 D446 D447 I448 V453 F456 E457 K458 E459 F460

Y461 L462 F463 L464 N467 G468 Q469 H470 L471 L472 E473 H474 I475 R476 T477 T478 K479 D480 L481 P482 N483 E484 D485 D486 K489 I491 F494 K495 K496 Q502

• Molecule 2: ATP synthase subunit beta

Chain D: 48% 47% • •

MSE HIS HIS HIS HIS HIS HIS HIS HIS HIS T2 R3 G4 M10 G11 P12 V13 V14 D15 V16 K17 F18 I26 Y27 L30 K31 I32 N38 V42 D43 I44 D45 L46 T47 L48 A51 L52 H53 L54 GLY D56 D57 T58 V59 R60 T61 I62 A63 M64 T67 D68 G69

L70 I71 M74 E75 V76 I77 D78 P82 I83 S84 V85 P86 V87 G88 E89 V90 T91 L92 G93 R94 N97 V98 E106 G107 D108 D112 A113 R114 H115 D116 P117 I118 H119 H120 F125 L128 A129 T130 E131 I134 L135 G138 I139 K140 V141 V142 D143 A146 P147

K150 G151 G152 K153 F157 G163 K164 T165 V166 L167 I168 Q169 E170 L171 I172 H173 N174 I175 A176 Q177 E178 G181 I182 S183 E190 R191 T192 R193 M202 T211 A212 M213 V214 F215 G216 Q217 M218 N219 G223 A224 R225 M226 R227 V228 A229 L230 T231 G232 L233 T234 M235 A236 E237
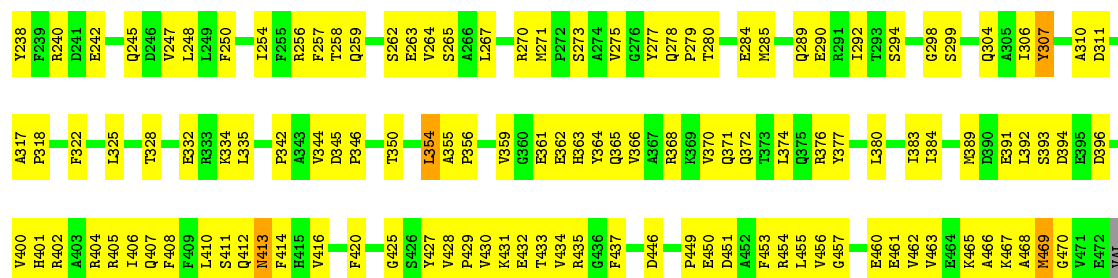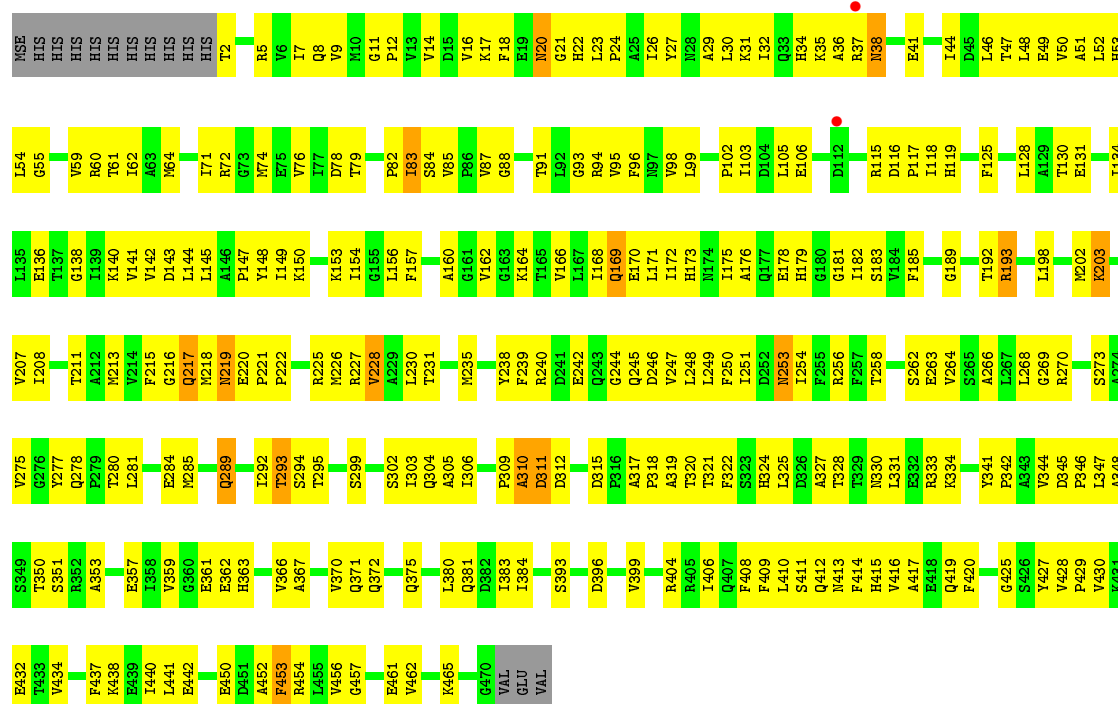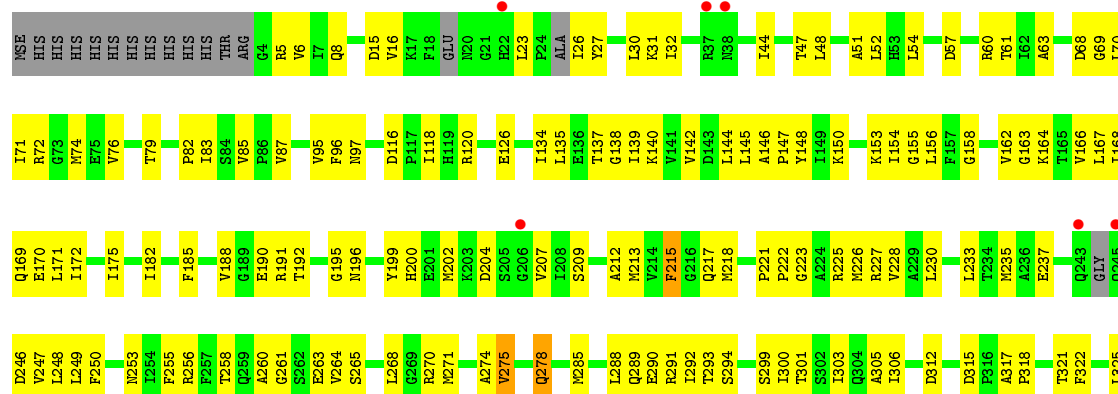
• Molecule 2: ATP synthase subunit beta

Chain E:

• Molecule 2: ATP synthase subunit beta

Chain F:

• Molecule 3: ATP synthase gamma chain

• Molecule 4: ATP synthase epsilon chain

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	233.40Å 233.40Å 303.96Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.99 – 3.90 19.99 – 3.70	Depositor EDS
% Data completeness (in resolution range)	99.0 (19.99-3.90) 99.7 (19.99-3.70)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.04 (at 3.71Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.250 , 0.282 0.259 , 0.290	Depositor DCC
R_{free} test set	1910 reflections (5.28%)	DCC
Wilson B-factor (Å²)	123.5	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol}(e/Å³), B_{sol}(Å²)	0.29 , 86.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning [2]	$<|L|> = 0.45$, $<L^2> = 0.27$	Xtriage
Outliers	0 of 44353 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	22656	wwPDB-VP
Average B, all atoms (Å²)	122.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.89% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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 (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.55	0/3496	0.75	0/4711
1	B	0.46	0/2853	0.70	0/3840
1	C	0.49	0/3367	0.74	3/4526 (0.1%)
2	D	0.50	0/3519	0.70	0/4735
2	E	0.54	0/3524	0.74	0/4751
2	F	0.45	0/3362	0.69	0/4504
3	G	0.54	0/1808	0.83	3/2435 (0.1%)
4	H	0.56	0/895	0.80	0/1202
All	All	0.51	0/22824	0.74	6/30704 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	2
2	D	0	2
2	F	0	1
3	G	0	1
All	All	0	6

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	484	GLU	N-CA-C	-6.31	93.97	111.00
3	G	217	LEU	CA-CB-CG	5.65	128.28	115.30
1	C	397	GLN	N-CA-C	-5.60	95.87	111.00
3	G	186	ARG	N-CA-C	-5.60	95.89	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	115	ILE	N-CA-C	5.53	125.93	111.00

There are no chirality outliers.

5 of 6 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	354	ARG	Peptide
1	C	401	ASP	Peptide
2	D	216	GLY	Peptide
2	D	391	GLU	Peptide
2	F	215	PHE	Peptide

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	3462	0	3344	321	0
1	B	2833	0	2533	243	0
1	C	3329	0	3032	283	0
2	D	3480	0	3309	272	0
2	E	3484	0	3345	268	0
2	F	3334	0	3069	202	0
3	G	1797	0	1665	192	0
4	H	890	0	833	87	0
5	A	5	0	0	3	0
5	B	5	0	0	1	0
5	D	5	0	0	0	0
5	E	5	0	0	0	0
6	F	27	0	12	1	0
All	All	22656	0	21142	1787	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 41.

The worst 5 of 1787 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:C:262:ASP:H	1:C:318:PHE:HB2	1.05	1.13
1:A:404:LYS:HG3	1:A:405:ALA:H	1.06	1.11
4:H:129:VAL:HG13	4:H:132:MSE:HA	1.33	1.09
2:F:139:ILE:HA	2:F:412:GLN:NE2	1.69	1.07
1:A:32:ILE:HG22	1:A:33:GLN:HG3	1.40	1.04

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	473/502 (94%)	429 (91%)	42 (9%)	2 (0%)	39	79
1	B	403/502 (80%)	357 (89%)	42 (10%)	4 (1%)	19	64
1	C	469/502 (93%)	411 (88%)	51 (11%)	7 (2%)	13	57
2	D	466/483 (96%)	414 (89%)	50 (11%)	2 (0%)	39	79
2	E	463/483 (96%)	418 (90%)	39 (8%)	6 (1%)	15	59
2	F	456/483 (94%)	406 (89%)	46 (10%)	4 (1%)	21	65
3	G	242/285 (85%)	193 (80%)	38 (16%)	11 (4%)	3	33
4	H	123/133 (92%)	108 (88%)	12 (10%)	3 (2%)	7	49
All	All	3095/3373 (92%)	2736 (88%)	320 (10%)	39 (1%)	15	59

5 of 39 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	371	GLN
1	C	354	ARG
2	D	393	SER
2	E	311	ASP
3	G	143	GLN

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	332/402 (83%)	309 (93%)	23 (7%)	19	59
1	B	242/402 (60%)	232 (96%)	10 (4%)	37	73
1	C	291/402 (72%)	274 (94%)	17 (6%)	25	64
2	D	333/385 (86%)	318 (96%)	15 (4%)	34	71
2	E	349/385 (91%)	334 (96%)	15 (4%)	35	72
2	F	309/385 (80%)	301 (97%)	8 (3%)	54	81
3	G	157/231 (68%)	148 (94%)	9 (6%)	25	65
4	H	78/104 (75%)	71 (91%)	7 (9%)	12	47
All	All	2091/2696 (78%)	1987 (95%)	104 (5%)	30	68

5 of 104 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	471	LEU
2	D	242	GLU
3	G	244	MSE
1	C	474	HIS
2	D	98	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 18 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	289	GLN
2	D	304	GLN
2	E	304	GLN
1	C	433	GLN
1	C	474	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)

5 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	$\#|Z| > 2$
5	SO4	A	700	-	4,4,4	0.31	0	6,6,6	0.31	0
5	SO4	B	700	-	4,4,4	0.28	0	6,6,6	0.28	0
5	SO4	D	700	-	4,4,4	0.21	0	6,6,6	0.15	0
5	SO4	E	700	-	4,4,4	0.13	0	6,6,6	0.17	0
6	ADP	F	600	-	24,29,29	1.06	1 (4%)	23,45,45	1.76	3 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	SO4	A	700	-	-	0/0/0/0	0/0/0/0
5	SO4	B	700	-	-	0/0/0/0	0/0/0/0
5	SO4	D	700	-	-	0/0/0/0	0/0/0/0
5	SO4	E	700	-	-	0/0/0/0	0/0/0/0
6	ADP	F	600	-	-	0/12/32/32	0/3/3/3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	600	ADP	C5-C4	3.27	1.47	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	F	600	ADP	N3-C2-N1	-6.55	123.72	128.87
6	F	600	ADP	C4'-O4'-C1'	2.21	111.98	109.64
6	F	600	ADP	N6-C6-N1	2.22	122.23	118.52

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	700	SO4	3	0
5	B	700	SO4	1	0
6	F	600	ADP	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	468/502 (93%)	-0.55	2 (0%)	93	90	63, 97, 156, 240	0
1	B	414/502 (82%)	-0.21	10 (2%)	62	50	92, 129, 236, 263	0
1	C	466/502 (92%)	-0.39	2 (0%)	93	90	86, 124, 177, 215	0
2	D	457/483 (94%)	-0.35	2 (0%)	93	90	70, 107, 165, 212	0
2	E	456/483 (94%)	-0.39	2 (0%)	93	90	71, 103, 155, 210	0
2	F	451/483 (93%)	-0.22	7 (1%)	74	64	95, 137, 164, 211	0
3	G	247/285 (86%)	-0.25	1 (0%)	93	90	80, 134, 182, 199	0
4	H	125/133 (93%)	0.05	5 (4%)	42	31	114, 143, 168, 191	0
All	All	3084/3373 (91%)	-0.33	31 (1%)	84	77	63, 119, 180, 263	0

The worst 5 of 31 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	243	GLN	5.9
2	D	2	THR	4.0
4	H	76	THR	4.0
2	F	420	PHE	3.9
1	B	142	VAL	3.5

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
5	SO4	A	700	5/5	0.80	0.51	4.16	184,186,190,192	0
5	SO4	E	700	5/5	0.76	0.34	2.09	185,189,190,191	0
5	SO4	B	700	5/5	0.57	0.38	1.18	187,190,191,194	0
6	ADP	F	600	27/27	0.79	0.34	0.55	173,198,203,203	0
5	SO4	D	700	5/5	0.84	0.25	-0.16	190,192,193,194	0

6.5 Other polymers (i)

There are no such residues in this entry.