WORLDWIDE PDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report ⓘ

Aug 29, 2023 – 04:36 AM EDT

PDB ID	:	3OE7
Title	:	Structure of four mutant forms of yeast f1 ATPase: gamma-I270T
Authors	:	Arsenieva, D.; Symersky, J.; Wang, Y.; Pagadala, V.; Mueller, D.M.
Deposited on	:	2010-08-12
Resolution	:	3.19 Å(reported)

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

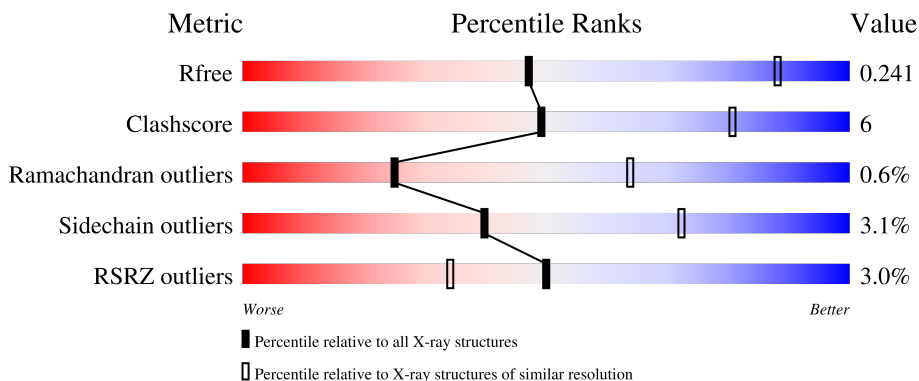|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.19 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	Percentile Ranks	Value
Rfree		0.241
Clashscore		6
Ramachandran outliers		0.6%
Sidechain outliers		3.1%
RSRZ outliers		3.0%

Worse   *Better*

▉ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
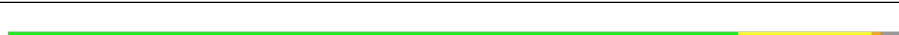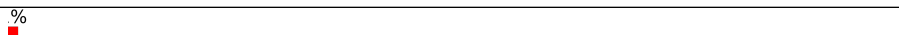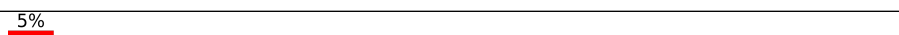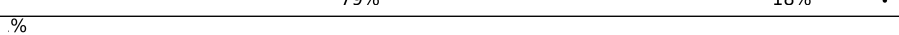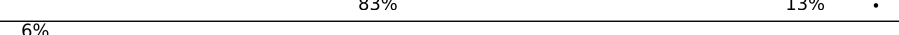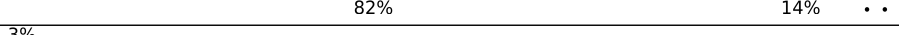
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of 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 <=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	78% 15% • 5%
1	B	510	.% 80% 14% • 5%
1	C	510	83% 11% • 5%
1	J	510	80% 14% • 6%
1	K	510	4% 78% 16% 5%

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Mol	Chain	Length	Quality of chain
1	L	510	79% 15% 5%
1	S	510	% 82% 11% 6%
1	T	510	4% 76% 18% 6%
1	U	510	6% 79% 15% 6%
2	D	484	82% 14%
2	E	484	3% 80% 16%
2	F	484	82% 15%
2	M	484	% 80% 16%
2	N	484	5% 79% 18%
2	O	484	% 83% 13%
2	V	484	6% 82% 14%
2	W	484	3% 82% 13%
2	X	484	4% 82% 14%
3	G	278	74% 20% 5%
3	P	278	10% 59% 24% 5% 12%
3	Y	278	8% 59% 12% 29%
4	H	137	4% 71% 16% 12%
4	Q	137	13% 55% 6% 39%
4	Z	137	7% 10% 89%
5	1	61	15% 38% 59%
5	I	61	61% 18% 21%
5	R	61	46% 5% 49%

2 Entry composition ⓘ

There are 8 unique types of molecules in this entry. The entry contains 72533 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	482	Total	C	N	O	S	0	0	0
			3664	2314	648	699	3			
1	B	483	Total	C	N	O	S	0	0	0
			3669	2317	649	700	3			
1	C	484	Total	C	N	O	S	0	0	0
			3674	2319	650	702	3			
1	J	481	Total	C	N	O	S	0	0	0
			3655	2309	646	697	3			
1	K	486	Total	C	N	O	S	0	0	0
			3694	2331	652	708	3			
1	L	482	Total	C	N	O	S	0	0	0
			3664	2314	648	699	3			
1	S	480	Total	C	N	O	S	0	0	0
			3651	2307	645	696	3			
1	T	481	Total	C	N	O	S	0	0	0
			3659	2311	647	698	3			
1	U	481	Total	C	N	O	S	0	0	0
			3659	2311	647	698	3			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	E	468	Total	C	N	O	S	0	0	0
			3536	2243	602	685	6			
2	F	469	Total	C	N	O	S	0	0	0
			3543	2247	603	687	6			
2	M	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			
2	N	470	Total	C	N	O	S	0	0	0
			3549	2250	604	689	6			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	468	Total 3538	C 2244	N 602	O 686	S 6	0	0	0
2	V	470	Total 3549	C 2250	N 604	O 689	S 6	0	0	0
2	W	467	Total 3531	C 2240	N 601	O 684	S 6	0	0	0
2	X	469	Total 3543	C 2247	N 603	O 687	S 6	0	0	0

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

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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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	265	Total 2042	C 1282	N 356	O 394	S 10	0	0	0
3	P	244	Total 1847	C 1159	N 322	O 357	S 9	0	0	0
3	Y	198	Total 1356	C 827	N 250	O 272	S 7	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	270	THR	ILE	engineered mutation	UNP P38077
P	270	THR	ILE	engineered mutation	UNP P38077
Y	270	THR	ILE	engineered mutation	UNP P38077

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	120	Total 775	C 484	N 135	O 154	S 2	0	0	0
4	Q	84	Total 449	C 271	N 88	O 90		0	0	0
4	Z	15	Total 75	C 45	N 15	O 15		0	0	0

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	48	Total 330	C 204	N 59	O 67	0	0	0
5	R	31	Total 173	C 107	N 32	O 34	0	0	0
5	1	25	Total 125	C 75	N 25	O 25	0	0	0

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

ANP

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	A	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	D	1	Total 1	Mg 1	0	0
7	F	1	Total 1	Mg 1	0	0
7	J	1	Total 1	Mg 1	0	0
7	K	1	Total 1	Mg 1	0	0
7	L	1	Total 1	Mg 1	0	0
7	M	1	Total 1	Mg 1	0	0
7	O	1	Total 1	Mg 1	0	0
7	S	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	V	1	Total 1	Mg 1	0	0
7	X	1	Total 1	Mg 1	0	0

- Molecule 8 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

PO4

O3

O⁻

O2 O⁻ — P = O O1

P

O⁻

O4
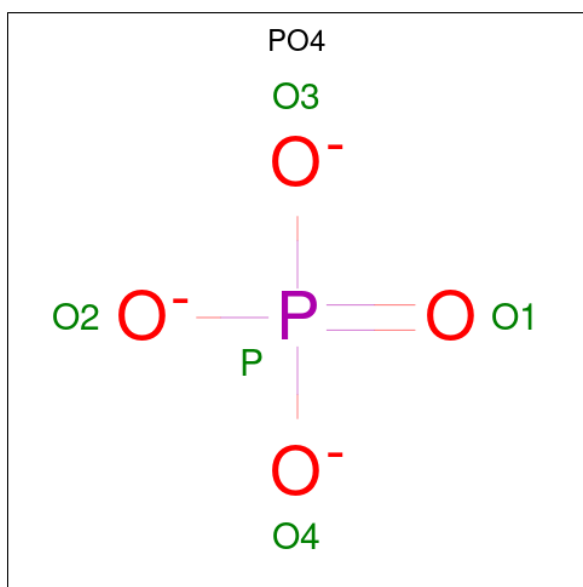
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	N	1	Total 5	O 4	P 1	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.
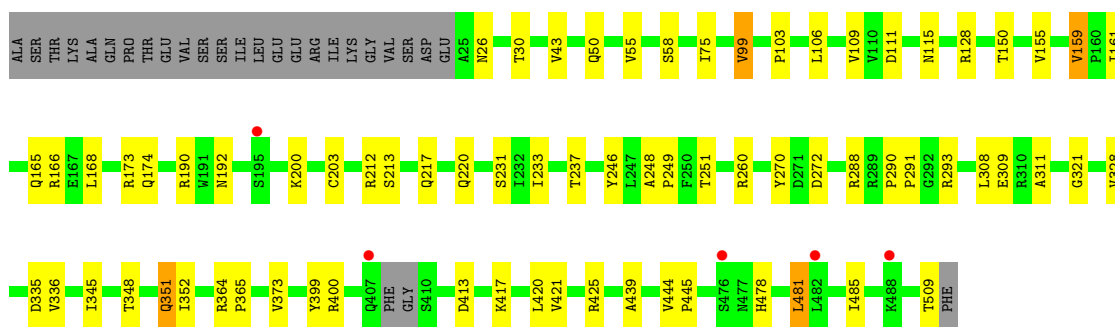
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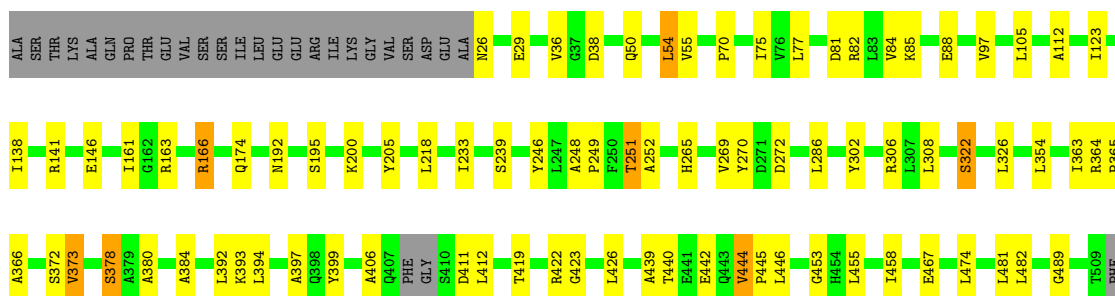
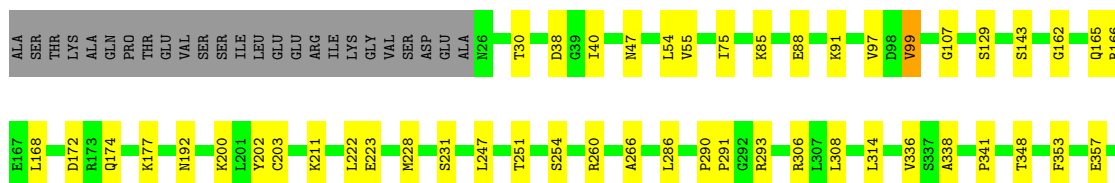- Molecule 1: ATP synthase subunit alpha

- Molecule 1: ATP synthase subunit alpha

R364 P365 Q407 F408 G409 S410 D411 A414 S415 T416 K417 Q418 R422 G453 L481 L495 K500 E504 T509 PHE

• Molecule 1: ATP synthase subunit alpha

Chain J:

80%   14%   6%

ALA SER THR LYS ALA GLN PRO THR GLU VAL SER SER ILE LEU GLU GLU ARG ILE GLY VAL SER ASP GLU ALA N26 E29 Q50 A51 E52 E53 L54 V55 P70 I75 V97 L105 I123 R142 E146 R163 R166 Q174 D183 L186

C203 V204 L218 H225 S231 T237 F250 E257 R260 H265 I268 D271 D272 R293 E294 R306 L307 L308 E309 R310 G321 S322 V328 Q332 V336 F353 L358 F359 Y360 K361 G362 I363 R364 P365 R375 Y399 V402 A406

GLN PHE GLY S410 A414 T419 L420 G423 L426 L429 T440 V444 P445 L446 I458 E467 S468 S469 K475 N479 E480 L481 S498 T503 F506 T509 PHE

• Molecule 1: ATP synthase subunit alpha

Chain K:

4%

78%   16%   5%

ALA SER THR LYS ALA GLN PRO THR GLU VAL SER SER ILE LEU GLU GLU ARG ILE LYS GLY V21 E24 A35 D38 R42 L46 I49 L54 V55 A65 L66 N67 L68 E69 P70 I75 D81 I96 V97 D98 V99 L106 V109 I117 S129

P140 R141 R142 P147 A154 R166 I169 Q174 R173 N192 S195 K200 C203 R212 V219 E223 Y230 I233 V234 T237 A242 P243 Y246 F250 T251 A252 R260 V269 D272 L273 S274 Q282 L283 S284 L285 L286

Y302 S305 R306 L307 L308 A311 A312 G321 S322 L323 T324 A325 L326 P327 V328 A338 Y339 I340 P341 I345 Q351 I363 I367 V382 Q407 PHE GLY SER D411 L412 D413 K417 L420 V421 R425 L429 L430 K431 E442 Q443 V444 P445 L446 N452

G453 H454 L455 D456 G457 L471 H478 I485 K488 S498 L499 T503 E504 S505 F506 V507 A508 T509 PHE

• Molecule 1: ATP synthase subunit alpha

Chain L:

79%   15%   5%

ALA SER THR LYS ALA GLN PRO THR GLU VAL SER SER ILE LEU GLU GLU ARG ILE LYS GLY VAL SER ASP GLU ALA N26 L27 I40 I49 V55 E56 K62 L68 E69 I75 V76 R82 V90 V99 P103 L109 I117 K134 V159 L168

Q174 N187 R190 W191 N192 K200 K211 R212 S213 L218 I233 A238 S239 A242 P243 P249 F250 T251 W258 Y270 L283 V300 R306 A311 L323 V336 T342 I345 T348 D349 G350 Q351 I352 F353 R364 P365 R375

V376 A380 K383 G390 Q398 E401 Q407 PHE GLY S410 D411 L412 T416 K417 Q418 T419 L420 V421 R425 L429 L446 N452 G453 H454 L455 D456 G457 I458 I463 S468 S472 E480 L481 E484 E490 L491 S492 L495 A508 T509 PHE

• Molecule 1: ATP synthase subunit alpha

Chain S:

• Molecule 1: ATP synthase subunit alpha

Chain T:

• Molecule 1: ATP synthase subunit alpha

Chain U:

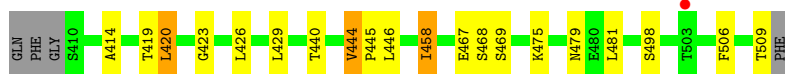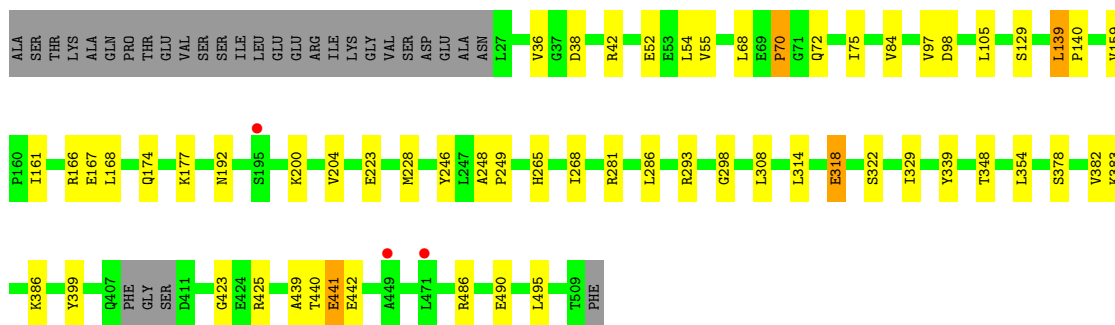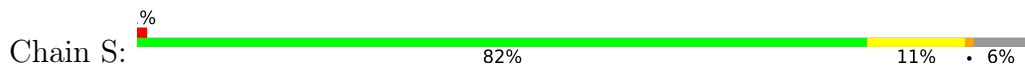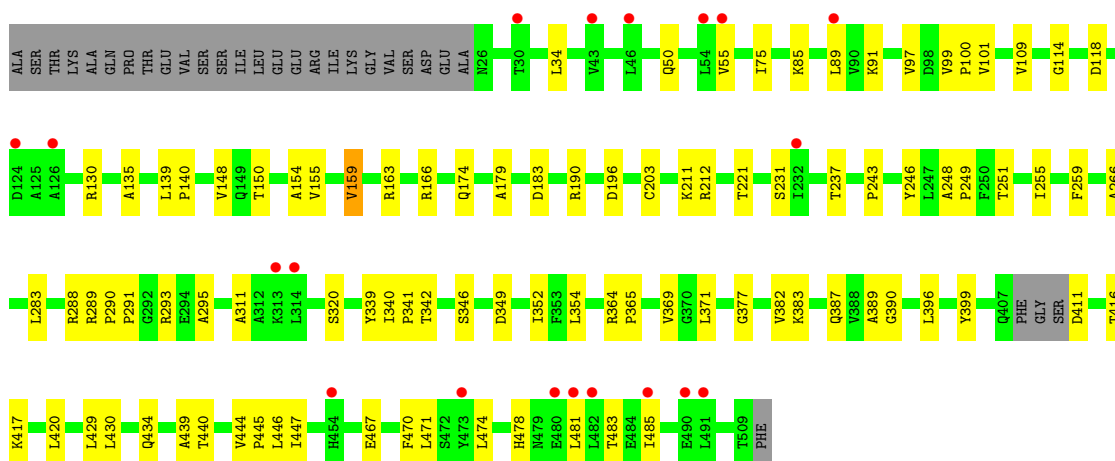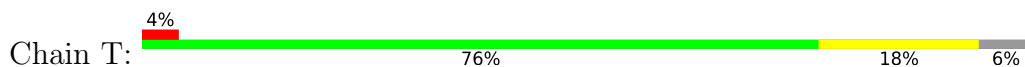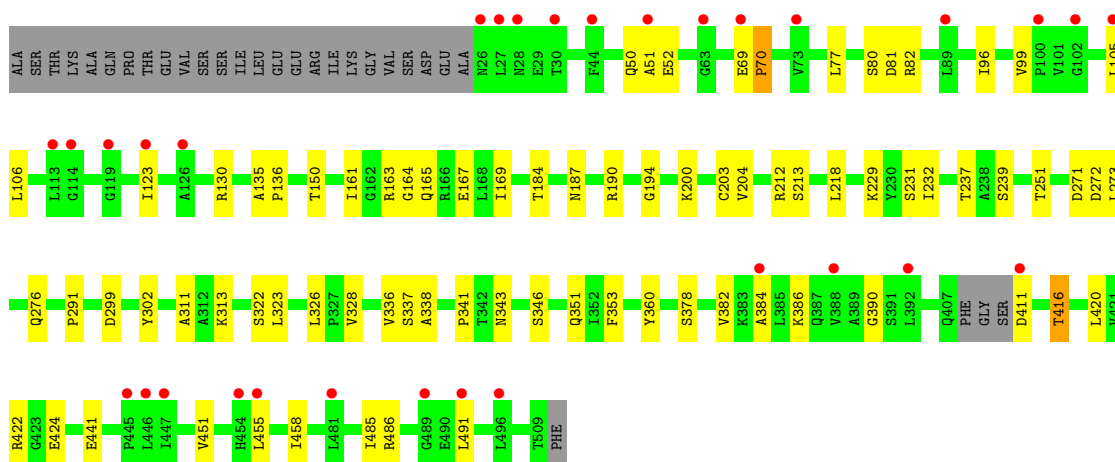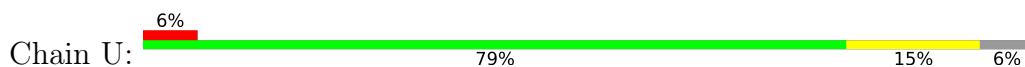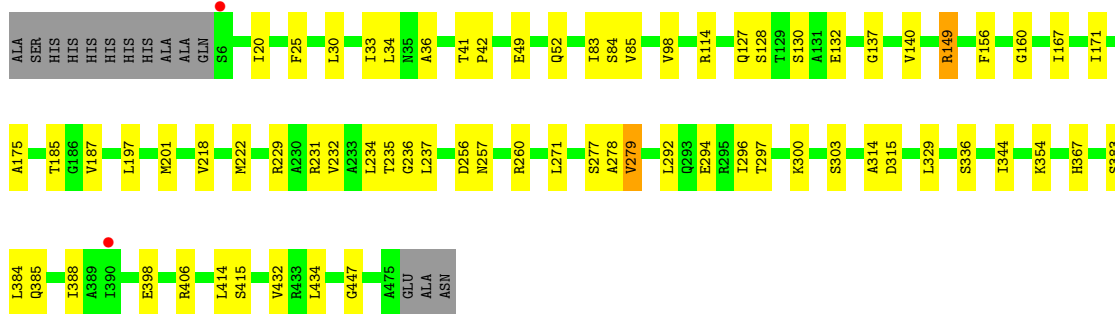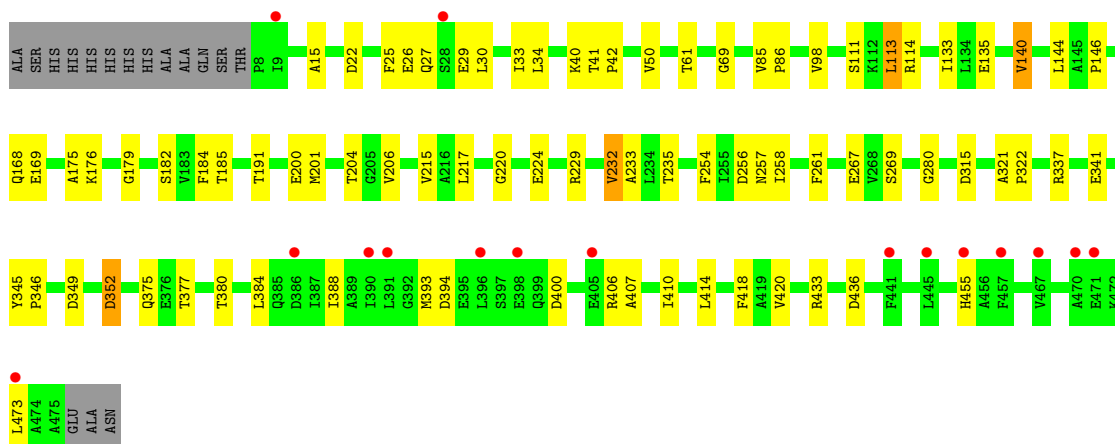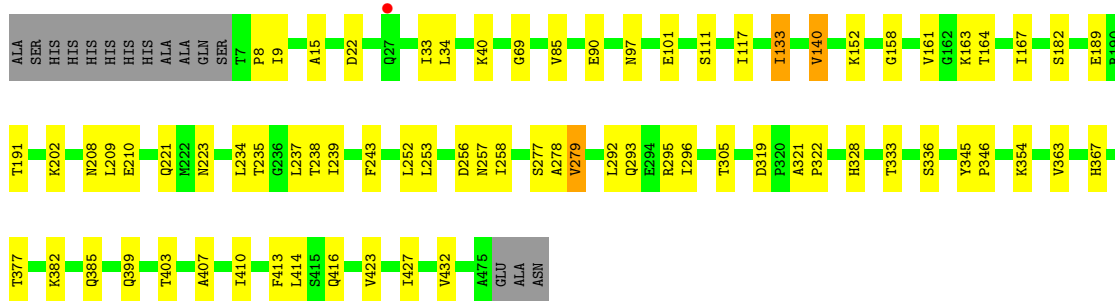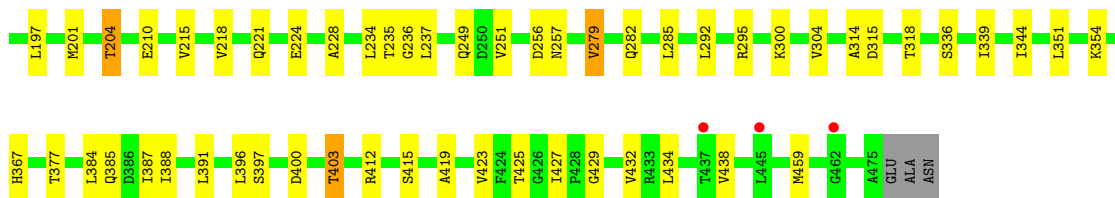• Molecule 2: ATP synthase subunit beta

Chain D: 82%   14%

ALA SER HIS HIS HIS HIS HIS ALA ALA GLN S6 I20 F25 L30 I33 L34 N35 A36 T41 P42 E49 Q52 I83 S84 V85 V98 R114 Q127 S128 T129 S130 A131 E132 G137 V140 R149 F156 G160 I167 I171

A175 T185 G186 V187 L197 M201 V218 M222 R229 A230 R231 V232 A233 L234 T235 G236 L237 D256 N257 R260 L271 S277 A278 V279 L292 Q293 E294 R295 I296 T297 K300 S303 A314 D315 L329 S336 I344 K354 H367 S383

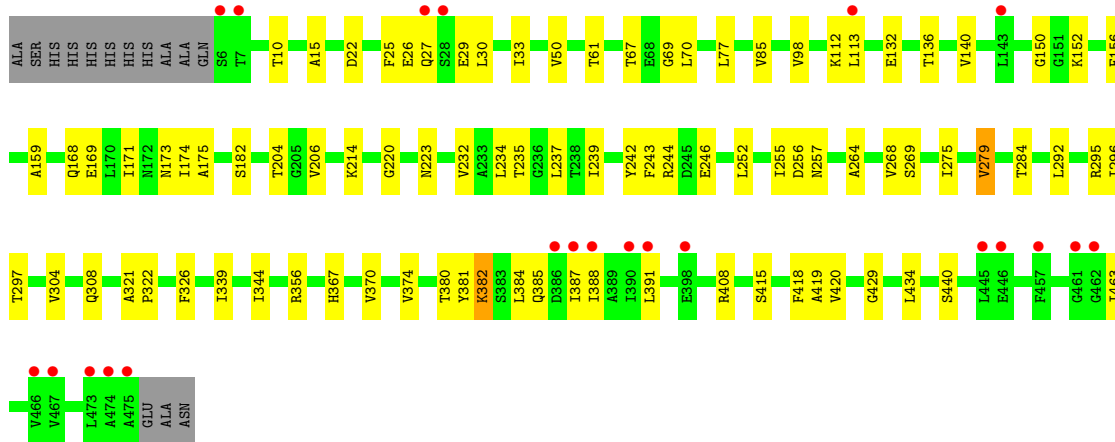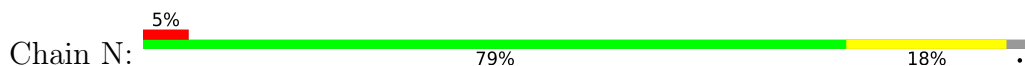L384 Q385 I388 A389 I390 E398 R406 L414 S415 V432 R433 L434 G447 A475 GLU ALA ASN

• Molecule 2: ATP synthase subunit beta

Chain E: 3%   80%   16%

ALA SER HIS HIS HIS HIS HIS ALA ALA GLN SER THR P8 I9 A15 D22 F25 E26 Q27 S28 E29 L30 I33 L34 K40 T41 P42 V50 T61 G69 V85 P86 V98 S111 K112 L113 R114 I133 L134 E135 V140 L144 A145 P146

Q168 E169 A175 K176 G179 S182 V183 F184 T185 T191 E200 M201 T204 G205 V206 V215 A216 L217 G220 E224 R229 V232 A233 L234 T235 F254 I255 D256 N257 I258 F261 E267 V268 S269 G280 D315 A321 P322 R337 E341

Y345 P346 D349 D352 Q375 E376 T377 T380 L384 Q385 D386 I387 I388 A389 I390 L391 G392 M393 D394 E395 L396 S397 E398 Q399 D400 E405 R406 A407 I410 L414 F418 A419 V420 R433 D436 F441 L445 H455 A456 F457 V467 A470 E471 K472
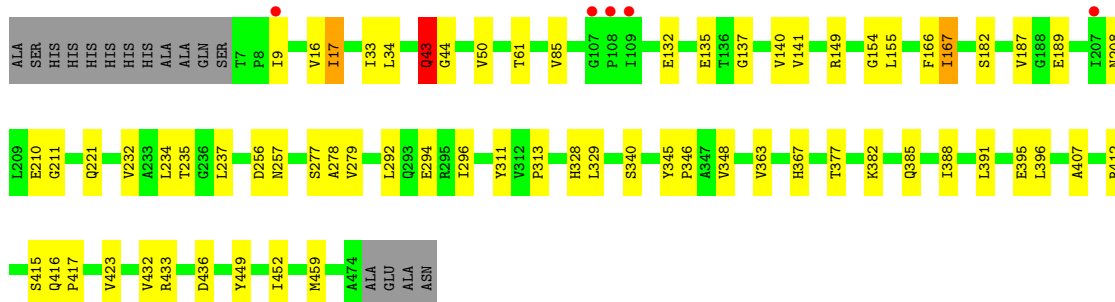
L473 A474 A475 GLU ALA ASN

• Molecule 2: ATP synthase subunit beta

Chain F: 82%   15%
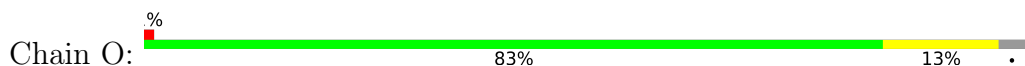
ALA SER HIS HIS HIS HIS HIS ALA ALA GLN SER T7 P8 I9 A15 D22 Q27 I33 L34 K40 G69 V85 E90 N97 E101 S111 I117 I133 V140 K152 G158 V161 G162 K163 T164 I167 S182 E189 R190

T191 K202 N208 L209 E210 Q221 M222 N223 L234 T235 G236 L237 T238 I239 F243 L252 L253 D256 N257 I258 S277 A278 V279 L292 Q293 E294 R295 I296 T305 D319 P320 A321 P322 H328 T333 S336 Y345 P346 K354 V363 H367

T377 K382 Q385 Q399 T403 A407 I410 F413 L414 S415 Q416 V423 I427 V432 A475 GLU ALA ASN
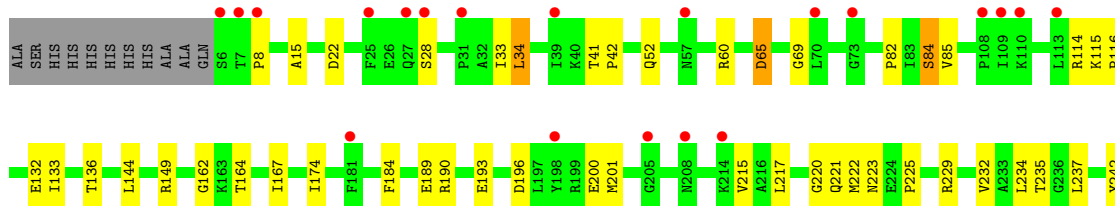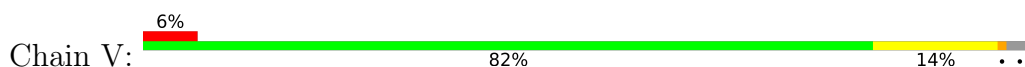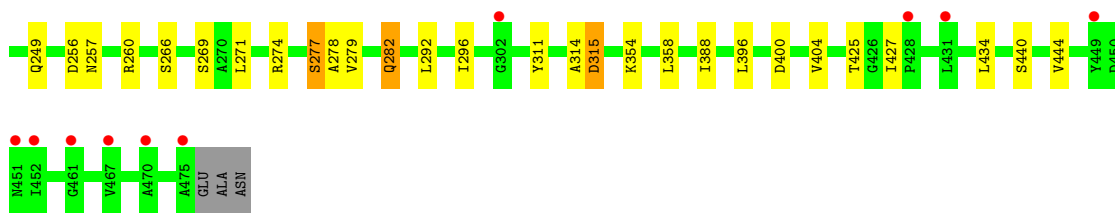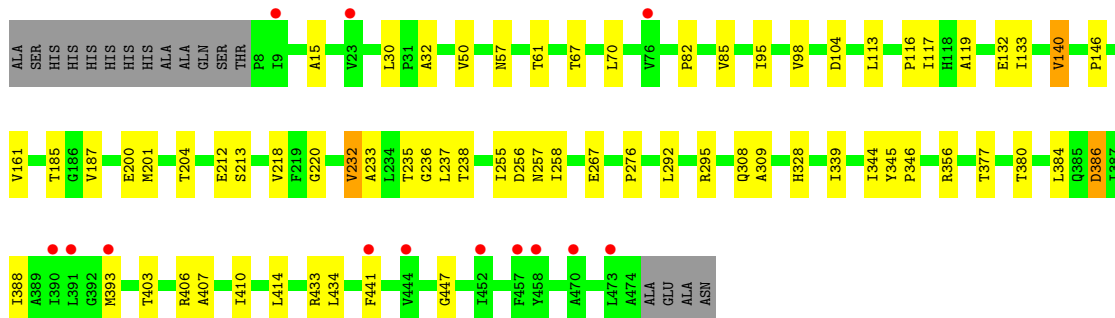
• Molecule 2: ATP synthase subunit beta

Chain M: %   80%   16%

ALA SER HIS HIS HIS HIS HIS ALA ALA GLN S6 T7 P8 V16 F25 E26 Q27 S28 E29 L30 I33 L34 T41 P42 H53 V59 R72 V85 I95 D104 A119 S128 G137 D142 L143 G160 I167 K176 S182 T191

L197 M201 T204 E210 V215 V218 Q221 E224 A228 L234 T235 G236 L237 Q249 D250 V251 D256 N257 V279 Q282 L285 L292 R295 K300 V304 A314 D315 T318 S336 I339 I344 L351 K354

H367 T377 L384 Q385 D386 I387 I388 L391 L396 S397 D400 T403 R412 S415 A419 V423 F424 T425 G426 I427 P428 G429 V432 R433 L434 T437 V438 L445 M459 G462 A475 GLU ALA ASN

• Molecule 2: ATP synthase subunit beta

Chain N:

5%

79% 18%

ALA SER HIS HIS HIS HIS HIS ALA ALA GLN S6 T7 T10 A15 D22 F25 E26 Q27 S28 E29 L30 I33 V50 T61 T67 E68 G69 L70 L77 V85 V98 K112 L113 E132 T136 V140 L143 G150 G151 K152 F156

A159 Q168 E169 L170 I171 N172 N173 I174 A175 S182 T204 G205 V206 K214 G220 N223 V232 A233 L234 T235 G236 L237 T238 I239 Y242 F243 R244 D245 E246 L252 I255 D256 N257 A264 V268 S269 I275 V279 T284 L292 R295 I296

T297 V304 Q308 A321 P322 F326 I339 I344 R356 H367 V370 V374 T380 Y381 K382 S383 L384 Q385 D386 I387 I388 A389 I390 L391 E398 R408 S415 F418 A419 V420 G429 L434 S440 L445 E446 F457 G461 G462 I463

V466 V467 L473 A474 A475 GLU ALA ASN

• Molecule 2: ATP synthase subunit beta

Chain O:
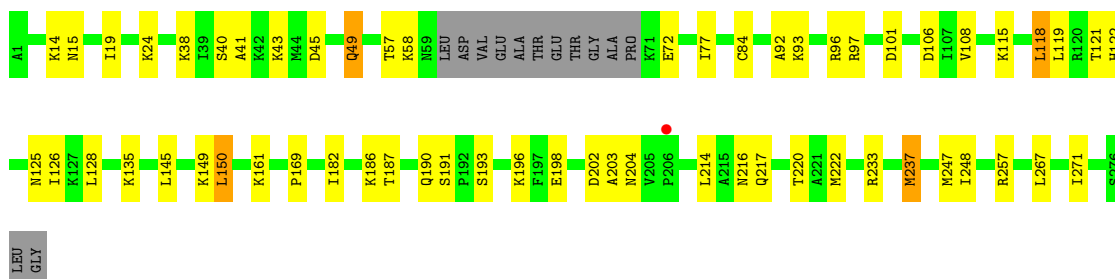
.%

83% 13%

ALA SER HIS HIS HIS HIS HIS ALA ALA GLN SER T7 P8 I9 V16 I17 I33 L34 Q43 G44 V50 T61 V85 G107 P108 I109 E132 E135 T136 G137 V140 V141 R149 G154 L155 F166 I167 S182 V187 G188 E189 I207 N208

L209 E210 G211 Q221 V232 A233 L234 T235 G236 L237 D256 N257 S277 A278 V279 L292 Q293 E294 R295 I296 Y311 V312 P313 H328 L329 S340 Y345 P346 A347 V348 V363 H367 T377 K382 Q385 I388 L391 E395 L396 A407 R412

S415 Q416 P417 V423 V432 R433 D436 Y449 I452 M459 A474 ALA GLU ALA ASN

• Molecule 2: ATP synthase subunit beta

Chain V:

6%

82% 14%

ALA SER HIS HIS HIS HIS HIS ALA ALA GLN S6 T7 P8 A15 D22 F25 E26 Q27 S28 P31 A32 I33 L34 I39 K40 T41 P42 Q52 N57 R60 D65 G69 L70 G73 P82 I83 S84 V85 P108 I109 K110 L113 R114 K115 P116

E132 I133 T136 L144 R149 G162 K463 T164 I167 I174 F181 F184 E189 R190 E193 D196 L197 Y198 R199 E200 M201 G205 N208 K214 V215 A216 L217 G220 Q221 M222 N223 E224 P225 R229 V232 A233 L234 T235 G236 L237 Y242

Q249 D256 N257 R260 S266 S269 A270 L271 R274 S277 A278 V279 Q282 L292 I296 G302 Y311 A314 D315 K354 L358 I388 L396 D400 V404 T425 G426 I427 P428 L431 L434 S440 V444 Y449 D450

N451 I452 G461 V467 A470 A475 GLU ALA ASN

• Molecule 2: ATP synthase subunit beta

Chain W:

3%

82% 13%

ALA SER HIS HIS HIS HIS HIS ALA ALA GLN SER THR P8 I9 A15 V23 L30 P31 A32 V50 N57 T61 T67 L70 V76 P82 V85 I95 V98 D104 L113 P116 I117 H118 A119 E132 I133 V140 P146

V161 T185 G186 V187 E200 M201 T204 E212 S213 V218 F219 G220 V232 A233 I234 T235 G236 L237 T238 I255 D256 N257 I258 E267 P276 L292 R295 Q308 A309 H328 I339 I344 Y345 P346 R356 T377 T380 L384 Q385 D386 I387

I388 A389 I390 L391 G392 M393 T403 R406 A407 I410 L414 R433 L434 F441 V444 G447 I452 F457 Y458 A470 L473 A474 ALA GLU ALA ASN

• Molecule 2: ATP synthase subunit beta

Chain X:

4%

82% 14%

ALA SER HIS HIS HIS HIS HIS ALA ALA GLN SER T7 P8 I9 A15 D22 F25 E26 Q27 S28 E29 L30 P31 A32 I33 L34 N57 G69 L77 D78 V85 P86 E90 I96 N97 E105 K110 S111 K112 S128 G162 F166 I167 L170

K176 A177 H178 G179 G180 F181 V187 G188 E189 R190 T191 R192 L197 M201 N208 L209 E210 G211 L217 V218 F219 G220 Q221 M222 N223 R231 L234 T235 G236 L237 D250 I255 D256 N257 R260 S269 L272 P276 V279 Q282 E294 R295 I296

T297 T298 T299 K300 S303 V307 Q308 A314 A321 P322 L335 I339 I344 Y345 P346 A347 L351 D359 V363 S372 L384 Q385 I390 R408 R412 A475 GLU ALA ASN

• Molecule 3: ATP synthase subunit gamma

Chain G:

74% 20% 5%

A1 K14 N15 I19 K24 K38 I39 S40 A41 K42 K43 M44 D45 Q49 T57 K58 N59 LEU ASP VAL GLU ALA THR GLU THR GLY ALA PRO K71 E72 I77 C84 A92 K93 R96 R97 D101 D106 I107 V108 K15 L118 L119 R120 T121 H122

N125 I126 K127 L128 K135 L145 K149 L150 K161 P169 I182 K186 T187 Q190 S191 P192 S193 K196 F197 E198 D202 A203 N204 V205 P206 L214 A215 N216 Q217 T220 A221 M222 R233 M237 M247 I248 R257 L267 I271 S276

LEU GLY

• 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:

D80 S81 Q82 L83 C84 V85 I88 E89 A90 PHE PRO LEU GLU SER PHE S97 K109 LYS ASN VAL SER SER ASP ALA ARG GLU ALA ALA GLU ALA ILE Q126 L137 LYS

• Molecule 4: ATP synthase subunit delta

7%

Chain Z: 10% 89%

GLU ALA ALA ALA ALA SER SER GLY LEU LYS LEU GLN PHE ALA LEU PRO HIS GLU THR LEU TYR SER GLY SER GLU VAL THR GLN VAL ASN LEU PRO ALA LYS SER GLY ARG ILE GLY VAL LEU ALA ASN HIS VAL PRO THR VAL GLU GLN LEU LEU PRO GLY VAL VAL GLU VAL MET GLU

GLY SER ASN SER LYS PHE ILE SER GLY GLY PHE ALA THR VAL GLN PRO ASP SER GLN LEU CYS VAL THR ALA ILE GLU GLU ALA PHE PRO LEU GLU GLU SER PHE SER GLN GLU ASN ILE LYS ASN LEU LEU ALA GLU ALA LYS LYS ASN VAL SER SER ASP ALA ARG GLU ALA A121

A124 I125 Q126 V127 E128 V129 L130 E131 N132 L133 Q134 S135 VAL LEU LYS

• Molecule 5: ATP synthase subunit epsilon

Chain I: 61% 18% 21%

SER ALA TRP ARG LYS ALA GLY I8 L14 A20 I21 R22 S23 SER LEU LYS T27 E28 L29 Q30 S33 R37 N49 GLY THR ALA A53 S54 E55 P56 T57 K61

• Molecule 5: ATP synthase subunit epsilon

Chain R: 46% 5% 49%

SER ALA TRP ARG LYS ALA GLY ILE SER Y10 R22 SER SER LEU LYS THR GLU LEU Q30 T31 A32 Y47 LYS ASN GLY THR ALA ALA SER GLU PRO THR PRO ILE THR LYS

• Molecule 5: ATP synthase subunit epsilon

15%

Chain 1: 38% 59%

SER ALA TRP ARG LYS ALA GLY ILE S9 Y10 A11 A12 Y13 L14 N15 V16 A17 A18 Q19 A20 I21 ARG SER SER LEU LYS THR GLU LEU GLN THR ALA SER V34 Q39 T40 T45 GLN TYR LYS ASN GLY THR ALA ALA SER GLU PRO THR PRO ILE THR LYS

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.03Å 292.21Å 189.05Å 90.00° 101.82° 90.00°	Depositor
Resolution (Å)	20.00 – 3.19 49.47 – 3.19	Depositor EDS
% Data completeness (in resolution range)	95.4 (20.00-3.19) 95.4 (49.47-3.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.189 , 0.245 0.188 , 0.241	Depositor DCC
R_{free} test set	9702 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å^2)	84.9	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 53.7	EDS
L-test for twinning[2]	$< |L| > = 0.47, < L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	72533	wwPDB-VP
Average B, all atoms (Å^2)	103.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.25% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: ANP, MG, 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	0.43	0/3718	0.60	0/5032
1	B	0.38	0/3723	0.56	0/5039
1	C	0.39	0/3729	0.56	0/5048
1	J	0.36	0/3709	0.54	0/5020
1	K	0.37	0/3748	0.53	0/5073
1	L	0.40	0/3718	0.57	0/5032
1	S	0.36	0/3705	0.54	0/5014
1	T	0.36	0/3713	0.51	0/5025
1	U	0.37	0/3713	0.52	0/5025
2	D	0.41	0/3605	0.58	0/4889
2	E	0.41	0/3592	0.56	1/4870 (0.0%)
2	F	0.39	0/3599	0.56	0/4881
2	M	0.40	0/3605	0.56	0/4889
2	N	0.38	0/3605	0.53	0/4889
2	O	0.37	0/3594	0.55	0/4874
2	V	0.37	0/3605	0.53	0/4889
2	W	0.37	0/3587	0.53	0/4863
2	X	0.37	0/3599	0.53	0/4881
3	G	0.39	0/2067	0.54	0/2782
3	P	0.36	0/1865	0.52	0/2508
3	Y	0.32	0/1361	0.46	0/1843
4	H	0.40	0/783	0.54	0/1072
4	Q	0.34	0/448	0.51	0/614
4	Z	0.31	0/74	0.44	0/102
5	1	0.32	0/123	0.50	0/169
5	I	0.44	0/332	0.59	0/452
5	R	0.38	0/173	0.53	0/238
All	All	0.38	0/73093	0.55	1/99013 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	113	LEU	CA-CB-CG	5.21	127.27	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3664	0	3747	47	0
1	B	3669	0	3752	41	0
1	C	3674	0	3756	33	0
1	J	3655	0	3739	43	0
1	K	3694	0	3774	51	0
1	L	3664	0	3747	43	0
1	S	3651	0	3739	35	0
1	T	3659	0	3745	49	0
1	U	3659	0	3745	46	0
2	D	3549	0	3620	42	0
2	E	3536	0	3610	42	0
2	F	3543	0	3616	45	0
2	M	3549	0	3620	54	0
2	N	3549	0	3621	54	0
2	O	3538	0	3610	38	0
2	V	3549	0	3620	48	0
2	W	3531	0	3605	41	0
2	X	3543	0	3616	43	0
3	G	2042	0	2102	33	0
3	P	1847	0	1873	43	0
3	Y	1356	0	1262	15	0
4	H	775	0	640	19	0
4	Q	449	0	240	4	0
4	Z	75	0	38	0	0
5	1	125	0	66	1	0
5	I	330	0	260	8	0
5	R	173	0	101	0	0
6	A	31	0	13	1	0
6	B	31	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	31	0	13	1	0
6	D	31	0	13	4	0
6	F	31	0	13	0	0
6	J	31	0	13	0	0
6	K	31	0	13	0	0
6	L	31	0	13	1	0
6	M	31	0	13	2	0
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	1	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
8	N	5	0	0	0	0
All	All	72533	0	73059	852	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 6.

The worst 5 of 852 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)
3:G:96:ARG:HE	3:G:121:THR:HG21	1.25	0.98
2:E:85:VAL:HG11	2:E:235:THR:HG23	1.47	0.96
3:P:180:LYS:HZ3	3:P:220:THR:HB	1.33	0.94
1:K:99:VAL:HG11	1:K:251:THR:HB	1.48	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:85:VAL:HG11	2:F:235:THR:HG23	1.51	0.92

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	478/510 (94%)	456 (95%)	20 (4%)	2 (0%)	34	69
1	B	479/510 (94%)	457 (95%)	22 (5%)	0	100	100
1	C	482/510 (94%)	460 (95%)	21 (4%)	1 (0%)	47	79
1	J	477/510 (94%)	460 (96%)	15 (3%)	2 (0%)	34	69
1	K	482/510 (94%)	458 (95%)	21 (4%)	3 (1%)	25	64
1	L	478/510 (94%)	454 (95%)	22 (5%)	2 (0%)	34	69
1	S	476/510 (93%)	454 (95%)	21 (4%)	1 (0%)	47	79
1	T	477/510 (94%)	452 (95%)	22 (5%)	3 (1%)	25	64
1	U	477/510 (94%)	447 (94%)	28 (6%)	2 (0%)	34	69
2	D	468/484 (97%)	444 (95%)	22 (5%)	2 (0%)	34	69
2	E	466/484 (96%)	437 (94%)	29 (6%)	0	100	100
2	F	467/484 (96%)	436 (93%)	29 (6%)	2 (0%)	34	69
2	M	468/484 (97%)	442 (94%)	23 (5%)	3 (1%)	25	64
2	N	468/484 (97%)	437 (93%)	29 (6%)	2 (0%)	34	69
2	O	466/484 (96%)	441 (95%)	23 (5%)	2 (0%)	34	69
2	V	468/484 (97%)	424 (91%)	40 (8%)	4 (1%)	17	56
2	W	465/484 (96%)	442 (95%)	23 (5%)	0	100	100
2	X	467/484 (96%)	439 (94%)	25 (5%)	3 (1%)	25	64
3	G	261/278 (94%)	244 (94%)	13 (5%)	4 (2%)	10	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	P	232/278 (84%)	202 (87%)	22 (10%)	8 (3%)	3	24
3	Y	186/278 (67%)	173 (93%)	12 (6%)	1 (0%)	29	67
4	H	110/137 (80%)	100 (91%)	10 (9%)	0	100	100
4	Q	74/137 (54%)	58 (78%)	11 (15%)	5 (7%)	1	9
4	Z	13/137 (10%)	10 (77%)	2 (15%)	1 (8%)	1	6
5	1	21/61 (34%)	18 (86%)	2 (10%)	1 (5%)	2	17
5	I	42/61 (69%)	32 (76%)	7 (17%)	3 (7%)	1	8
5	R	27/61 (44%)	22 (82%)	3 (11%)	2 (7%)	1	7
All	All	9475/10374 (91%)	8899 (94%)	517 (6%)	59 (1%)	25	64

5 of 59 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	G	202	ASP
1	J	414	ALA
2	M	28	SER
3	P	156	ALA
3	P	275	SER

5.3.2   Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/412 (94%)	373 (96%)	15 (4%)	32	67
1	B	388/412 (94%)	375 (97%)	13 (3%)	37	70
1	C	389/412 (94%)	378 (97%)	11 (3%)	43	74
1	J	387/412 (94%)	375 (97%)	12 (3%)	40	72
1	K	392/412 (95%)	387 (99%)	5 (1%)	69	87
1	L	388/412 (94%)	371 (96%)	17 (4%)	28	64
1	S	387/412 (94%)	379 (98%)	8 (2%)	53	79
1	T	388/412 (94%)	374 (96%)	14 (4%)	35	69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	U	388/412 (94%)	381 (98%)	7 (2%)	59	82
2	D	380/390 (97%)	370 (97%)	10 (3%)	46	76
2	E	378/390 (97%)	361 (96%)	17 (4%)	27	63
2	F	379/390 (97%)	366 (97%)	13 (3%)	37	70
2	M	380/390 (97%)	372 (98%)	8 (2%)	53	79
2	N	380/390 (97%)	370 (97%)	10 (3%)	46	76
2	O	379/390 (97%)	370 (98%)	9 (2%)	49	77
2	V	380/390 (97%)	374 (98%)	6 (2%)	62	84
2	W	378/390 (97%)	366 (97%)	12 (3%)	39	71
2	X	379/390 (97%)	374 (99%)	5 (1%)	69	87
3	G	223/236 (94%)	214 (96%)	9 (4%)	31	66
3	P	196/236 (83%)	172 (88%)	24 (12%)	5	22
3	Y	126/236 (53%)	117 (93%)	9 (7%)	14	47
4	H	62/112 (55%)	60 (97%)	2 (3%)	39	71
4	Q	9/112 (8%)	9 (100%)	0	100	100
5	I	24/48 (50%)	24 (100%)	0	100	100
5	R	3/48 (6%)	2 (67%)	1 (33%)	0	0
All	All	7551/8246 (92%)	7314 (97%)	237 (3%)	40	72

5 of 237 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	351	GLN
2	W	433	ARG
2	O	17	ILE
2	W	386	ASP
3	Y	269	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 51 such sidechains are listed below:

Mol	Chain	Res	Type
2	N	168	GLN
3	P	216	ASN
3	Y	15	ASN
2	O	52	GLN

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Mol	Chain	Res	Type
3	P	54	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 31 ligands modelled in this entry, 15 are monoatomic - leaving 16 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	#$\|Z\| > 2$
8	PO4	N	800	-	4,4,4	0.88	0	6,6,6	0.47	0
6	ANP	O	600	7	29,33,33	1.73	8 (27%)	31,52,52	1.89	9 (29%)
6	ANP	V	600	7	29,33,33	1.81	6 (20%)	31,52,52	2.03	8 (25%)
6	ANP	A	600	7	29,33,33	1.95	9 (31%)	31,52,52	1.70	8 (25%)
6	ANP	D	600	7	29,33,33	1.80	7 (24%)	31,52,52	1.76	8 (25%)
6	ANP	M	600	7	29,33,33	1.76	7 (24%)	31,52,52	2.03	6 (19%)
6	ANP	L	600	7	29,33,33	1.76	7 (24%)	31,52,52	1.94	9 (29%)
6	ANP	C	600	7	29,33,33	1.71	7 (24%)	31,52,52	1.85	7 (22%)
6	ANP	S	600	7	29,33,33	1.82	7 (24%)	31,52,52	1.95	8 (25%)
6	ANP	T	600	7	29,33,33	1.90	8 (27%)	31,52,52	1.88	8 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	ANP	B	600	7	29,33,33	1.90	6 (20%)	31,52,52	1.96	6 (19%)
6	ANP	X	600	7	29,33,33	1.79	8 (27%)	31,52,52	2.04	8 (25%)
6	ANP	U	600	7	29,33,33	1.80	7 (24%)	31,52,52	2.01	8 (25%)
6	ANP	J	600	7	29,33,33	1.81	7 (24%)	31,52,52	2.00	6 (19%)
6	ANP	K	600	7	29,33,33	1.86	8 (27%)	31,52,52	1.91	8 (25%)
6	ANP	F	600	7	29,33,33	1.69	8 (27%)	31,52,52	1.77	7 (22%)

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	O	600	7	-	5/14/38/38	0/3/3/3
6	ANP	V	600	7	-	6/14/38/38	0/3/3/3
6	ANP	A	600	7	-	2/14/38/38	0/3/3/3
6	ANP	D	600	7	-	4/14/38/38	0/3/3/3
6	ANP	M	600	7	-	4/14/38/38	0/3/3/3
6	ANP	L	600	7	-	3/14/38/38	0/3/3/3
6	ANP	C	600	7	-	3/14/38/38	0/3/3/3
6	ANP	S	600	7	-	3/14/38/38	0/3/3/3
6	ANP	T	600	7	-	4/14/38/38	0/3/3/3
6	ANP	B	600	7	-	6/14/38/38	0/3/3/3
6	ANP	X	600	7	-	9/14/38/38	0/3/3/3
6	ANP	U	600	7	-	4/14/38/38	0/3/3/3
6	ANP	J	600	7	-	3/14/38/38	0/3/3/3
6	ANP	K	600	7	-	5/14/38/38	0/3/3/3
6	ANP	F	600	7	-	7/14/38/38	0/3/3/3

The worst 5 of 110 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	600	ANP	PG-N3B	4.69	1.75	1.63
6	T	600	ANP	PB-N3B	4.54	1.75	1.63
6	S	600	ANP	PG-N3B	4.51	1.75	1.63
6	A	600	ANP	PB-N3B	4.50	1.75	1.63
6	V	600	ANP	PG-N3B	4.49	1.75	1.63

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	X	600	ANP	O1G-PG-N3B	-6.32	102.46	111.77
6	J	600	ANP	O1G-PG-N3B	-6.02	102.90	111.77
6	B	600	ANP	O1G-PG-N3B	-6.00	102.94	111.77
6	V	600	ANP	O1G-PG-N3B	-5.95	103.00	111.77
6	M	600	ANP	O2B-PB-O1B	5.89	122.28	109.92

There are no chirality outliers.

5 of 68 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	600	ANP	PB-N3B-PG-O1G
6	A	600	ANP	PG-N3B-PB-O1B
6	B	600	ANP	PB-N3B-PG-O1G
6	B	600	ANP	PG-N3B-PB-O1B
6	B	600	ANP	C5'-O5'-PA-O2A

There are no ring outliers.

9 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	V	600	ANP	1	0
6	A	600	ANP	1	0
6	D	600	ANP	4	0
6	M	600	ANP	2	0
6	L	600	ANP	1	0
6	C	600	ANP	1	0
6	T	600	ANP	2	0
6	B	600	ANP	1	0
6	X	600	ANP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient

equivalents in the CSD to analyse the geometry.

Ligand ANP O 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP V 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP A 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP D 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP M 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP L 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP C 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP S 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP T 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP B 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP X 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP U 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP J 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP K 600

Bond lengths

Bond angles

Torsions

Rings

Ligand ANP F 600

Bond lengths

Bond angles

Torsions

Rings

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, 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	482/510 (94%)	-0.32	0	100	100	45, 64, 100, 166	0
1	B	483/510 (94%)	-0.06	5 (1%)	82	72	48, 92, 165, 195	0
1	C	484/510 (94%)	-0.18	2 (0%)	92	89	51, 75, 138, 181	0
1	J	481/510 (94%)	-0.14	1 (0%)	95	94	59, 93, 137, 181	0
1	K	486/510 (95%)	0.03	18 (3%)	41	26	61, 107, 166, 182	0
1	L	482/510 (94%)	-0.22	2 (0%)	92	89	47, 68, 123, 164	0
1	S	480/510 (94%)	-0.08	3 (0%)	89	83	72, 106, 140, 186	0
1	T	481/510 (94%)	0.21	19 (3%)	38	25	91, 131, 153, 165	0
1	U	481/510 (94%)	0.27	31 (6%)	19	11	93, 133, 166, 194	0
2	D	470/484 (97%)	-0.26	2 (0%)	92	89	46, 72, 121, 172	0
2	E	468/484 (96%)	-0.02	16 (3%)	45	29	48, 85, 147, 186	0
2	F	469/484 (96%)	-0.17	1 (0%)	95	94	48, 84, 117, 161	0
2	M	470/484 (97%)	-0.14	6 (1%)	77	65	57, 84, 131, 172	0
2	N	470/484 (97%)	0.09	22 (4%)	31	19	64, 110, 165, 188	0
2	O	468/484 (96%)	-0.14	5 (1%)	80	69	53, 92, 128, 153	0
2	V	470/484 (97%)	0.30	30 (6%)	19	11	93, 139, 171, 189	0
2	W	467/484 (96%)	0.01	13 (2%)	53	37	76, 101, 137, 171	0
2	X	469/484 (96%)	0.11	17 (3%)	42	27	85, 121, 162, 187	0
3	G	265/278 (95%)	-0.15	1 (0%)	92	89	56, 90, 117, 134	0
3	P	244/278 (87%)	0.59	27 (11%)	5	3	64, 139, 185, 209	0
3	Y	198/278 (71%)	0.55	22 (11%)	5	3	98, 147, 190, 214	0
4	H	120/137 (87%)	0.09	6 (5%)	28	16	86, 115, 166, 176	0
4	Q	84/137 (61%)	0.90	18 (21%)	0	1	138, 163, 187, 198	0
4	Z	15/137 (10%)	1.94	9 (60%)	0	0	192, 201, 222, 222	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
5	1	25/61 (40%)	1.41	9 (36%)	0	0	176, 183, 194, 202	0
5	I	48/61 (78%)	-0.30	0	100	100	92, 112, 140, 157	0
5	R	31/61 (50%)	0.08	0	100	100	136, 153, 167, 178	0
All	All	9591/10374 (92%)	0.00	285 (2%)	50	34	45, 100, 160, 222	0

The worst 5 of 285 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	Q	83	LEU	5.4
2	M	6	SER	5.4
3	P	39	ILE	5.4
3	P	100	ASN	5.3
1	T	491	LEU	5.3

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 monosaccharides 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(Å²)	Q<0.9
7	MG	T	700	1/1	0.83	0.52	91,91,91,91	0
6	ANP	T	600	31/31	0.91	0.22	91,101,106,106	0
6	ANP	U	600	31/31	0.92	0.21	84,89,90,91	0
6	ANP	B	600	31/31	0.92	0.20	71,82,85,85	0
8	PO4	N	800	5/5	0.92	0.24	131,131,131,132	0
6	ANP	V	600	31/31	0.93	0.25	102,106,109,109	0
7	MG	D	700	1/1	0.93	0.36	64,64,64,64	0
6	ANP	X	600	31/31	0.94	0.24	93,94,96,97	0
7	MG	A	700	1/1	0.94	0.43	48,48,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
6	ANP	J	600	31/31	0.94	0.20	67,73,80,81	0
7	MG	F	700	1/1	0.94	0.44	65,65,65,65	0
7	MG	K	700	1/1	0.94	0.35	90,90,90,90	0
7	MG	S	700	1/1	0.94	0.41	77,77,77,77	0
6	ANP	K	600	31/31	0.94	0.17	90,97,99,100	0
7	MG	U	700	1/1	0.94	0.40	88,88,88,88	0
6	ANP	S	600	31/31	0.94	0.21	76,82,83,85	0
6	ANP	C	600	31/31	0.95	0.22	58,64,68,70	0
7	MG	L	700	1/1	0.95	0.33	53,53,53,53	0
6	ANP	F	600	31/31	0.95	0.26	66,70,78,78	0
7	MG	M	700	1/1	0.96	0.42	64,64,64,64	0
6	ANP	A	600	31/31	0.96	0.22	48,58,61,62	0
6	ANP	L	600	31/31	0.96	0.21	53,59,62,62	0
6	ANP	O	600	31/31	0.96	0.23	84,88,92,92	0
7	MG	B	700	1/1	0.96	0.41	72,72,72,72	0
7	MG	J	700	1/1	0.97	0.46	67,67,67,67	0
7	MG	C	700	1/1	0.97	0.45	58,58,58,58	0
6	ANP	D	600	31/31	0.97	0.22	62,65,68,69	0
7	MG	X	700	1/1	0.97	0.43	96,96,96,96	0
6	ANP	M	600	31/31	0.97	0.24	64,68,70,71	0
7	MG	O	700	1/1	0.98	0.43	83,83,83,83	0
7	MG	V	700	1/1	0.98	0.35	107,107,107,107	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
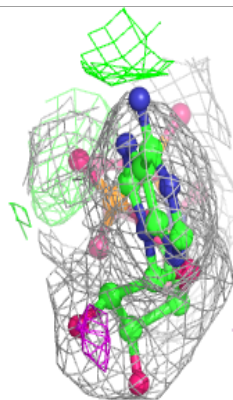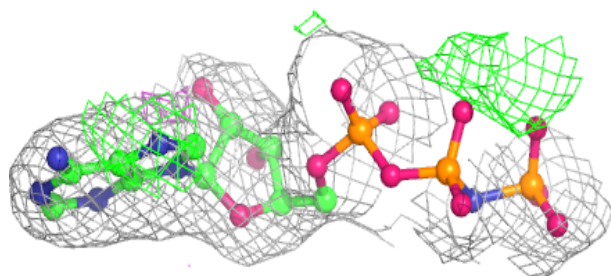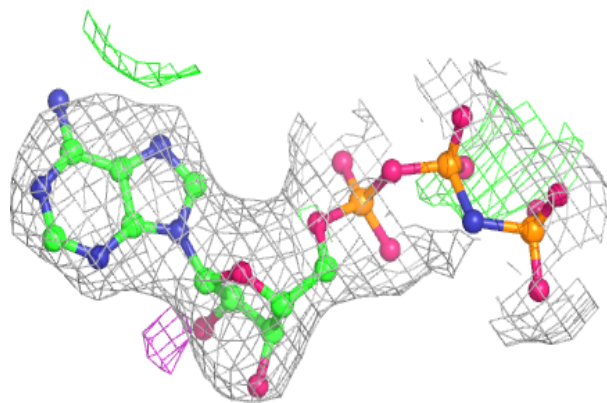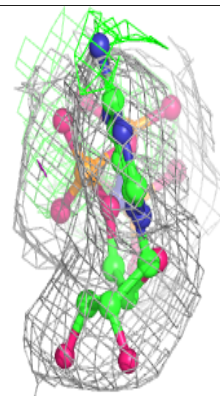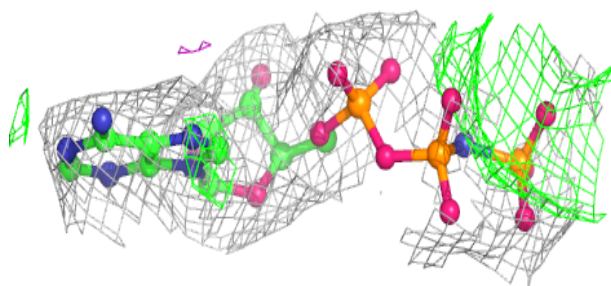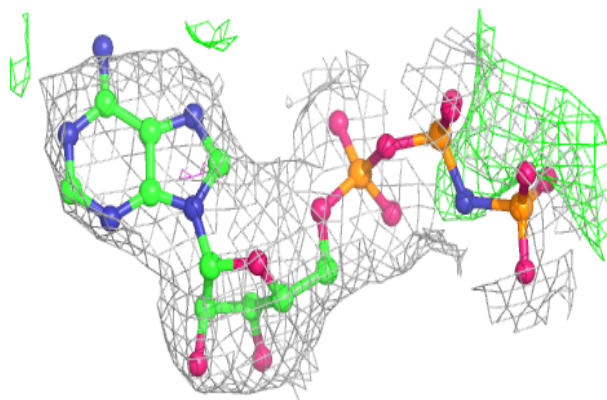
Electron density around ANP T 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
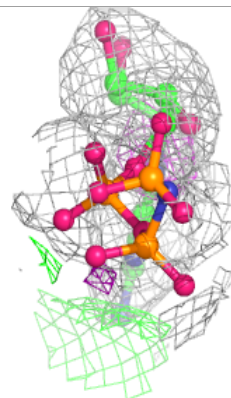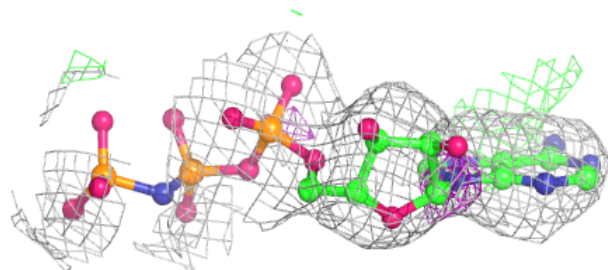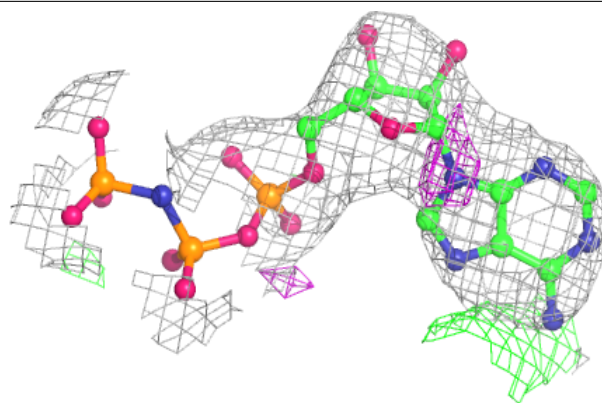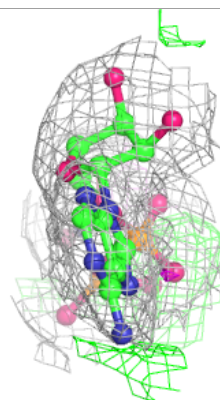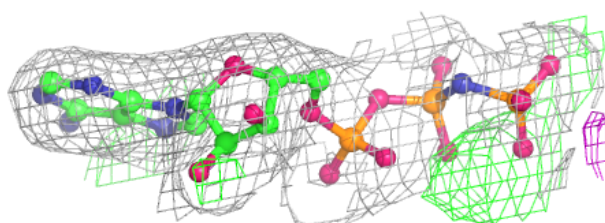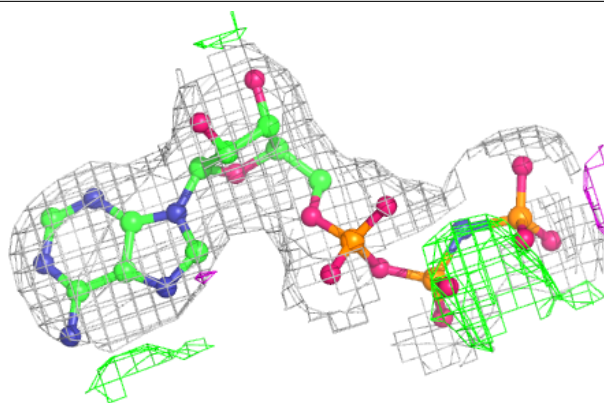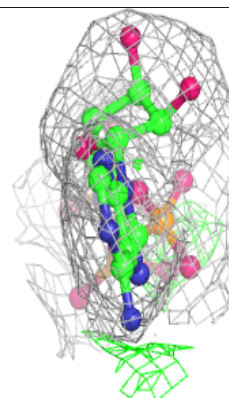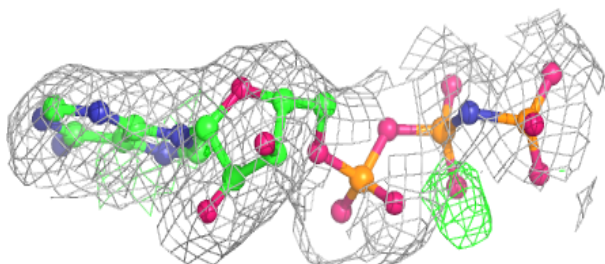

Electron density around ANP U 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around ANP B 600:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around ANP V 600:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
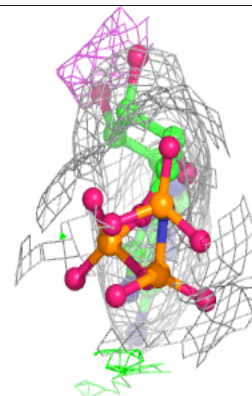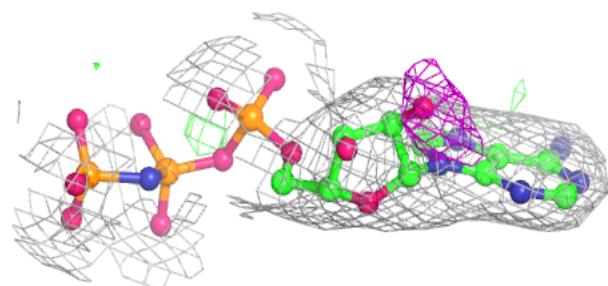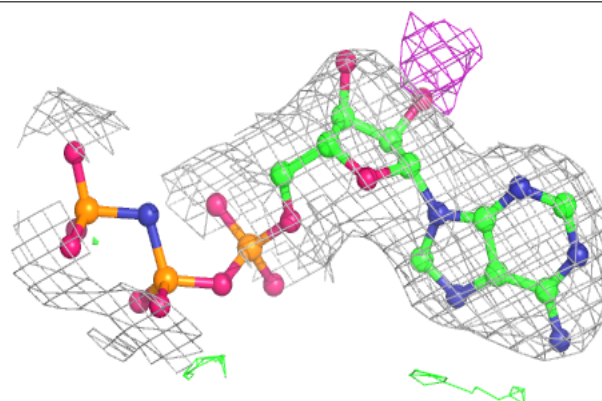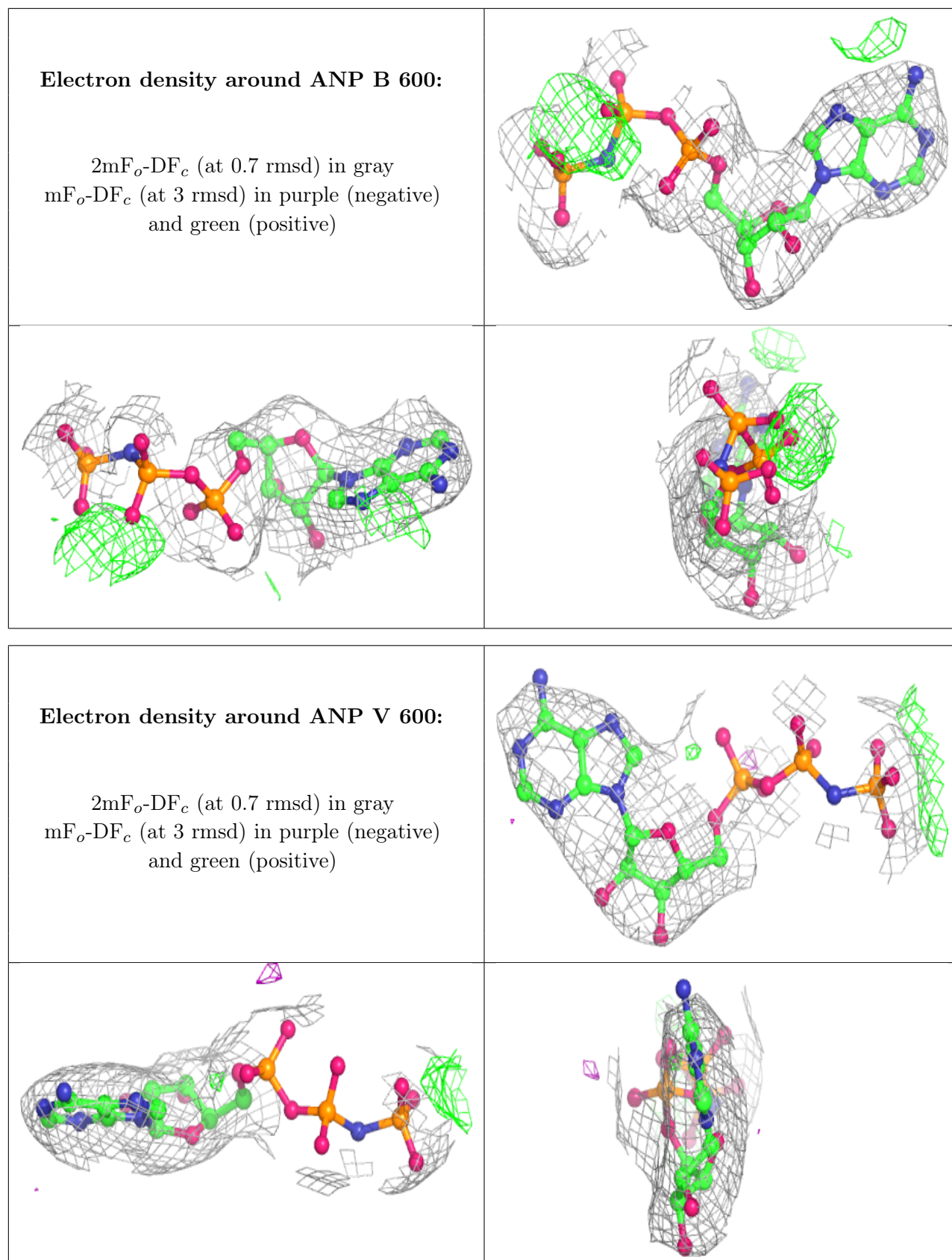
Electron density around ANP X 600:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
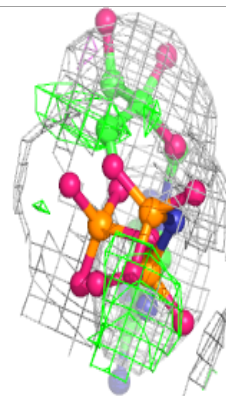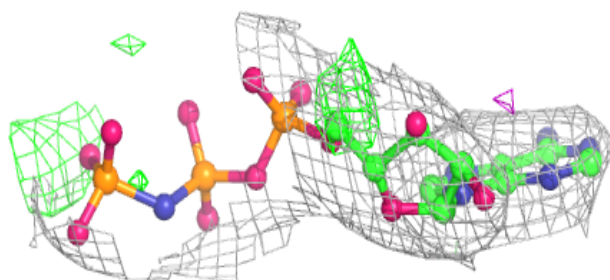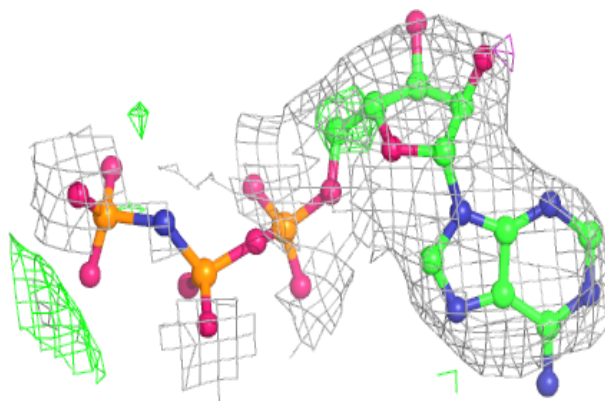
Electron density around ANP J 600:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
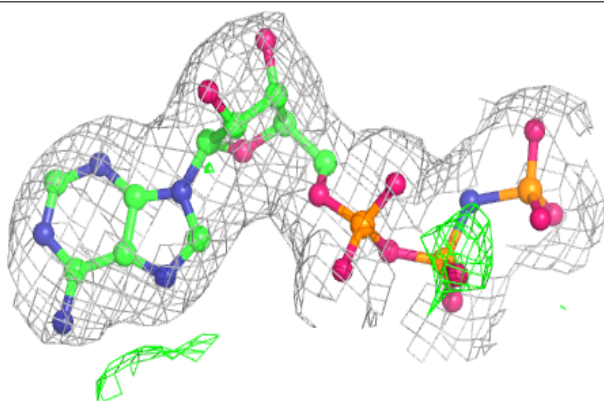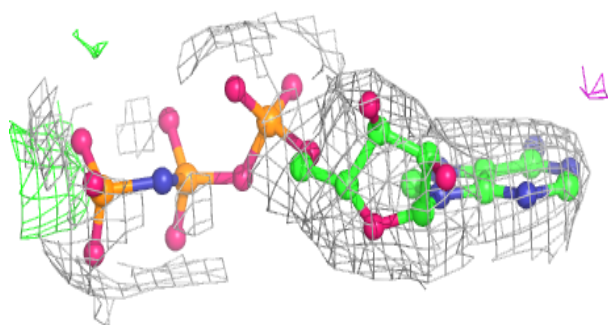$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
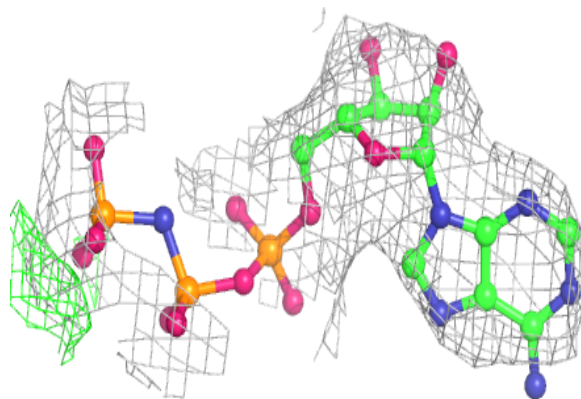and green (positive)
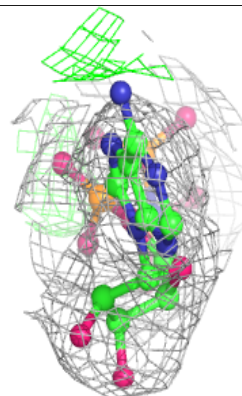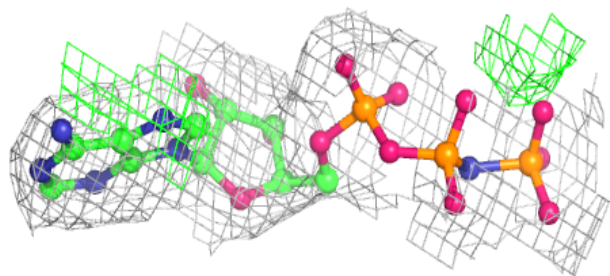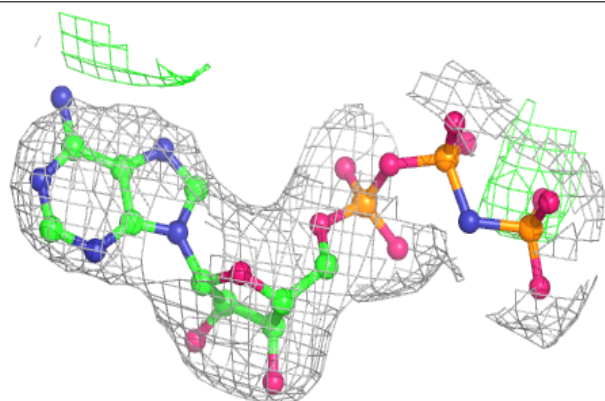
Electron density around ANP K 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
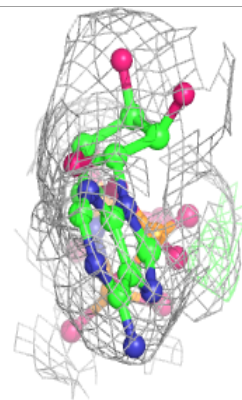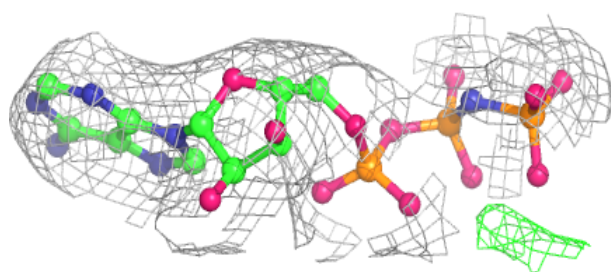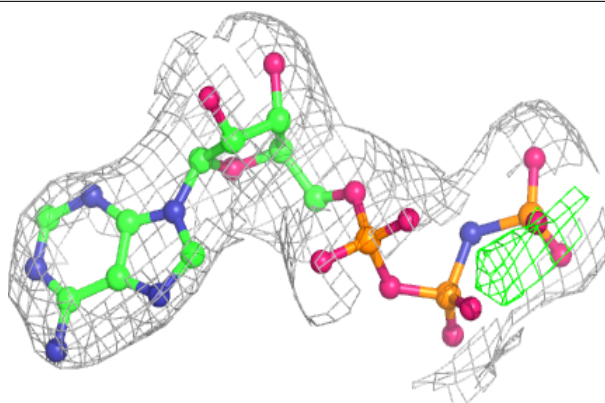
Electron density around ANP S 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
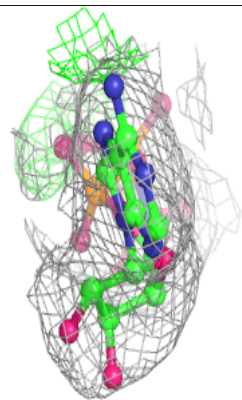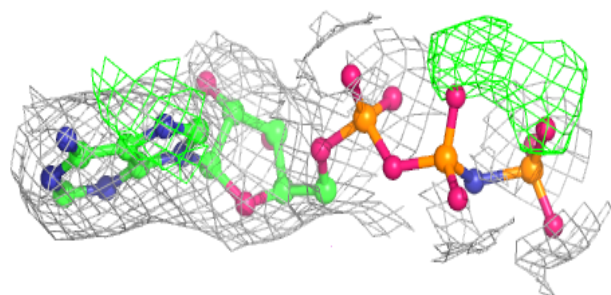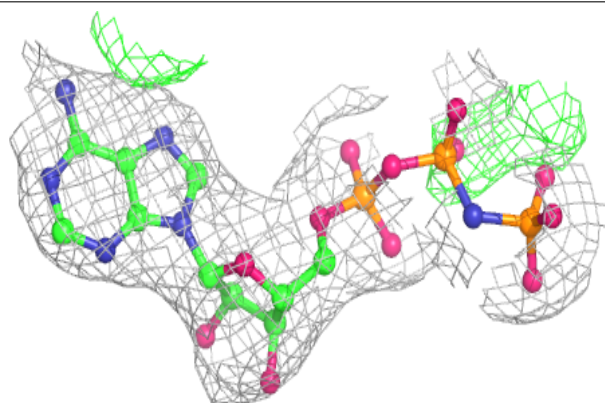
Electron density around ANP C 600:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around ANP F 600:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around ANP A 600:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around ANP L 600:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
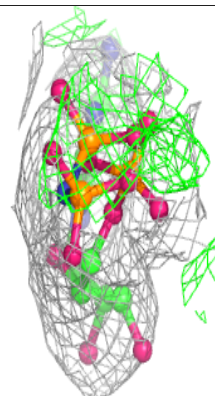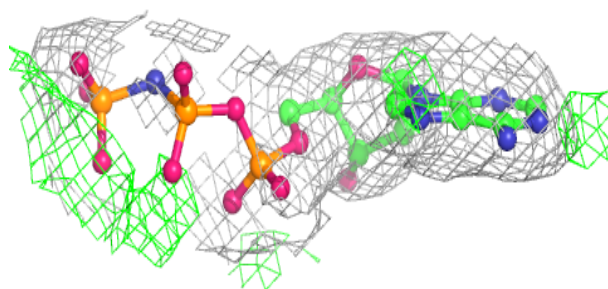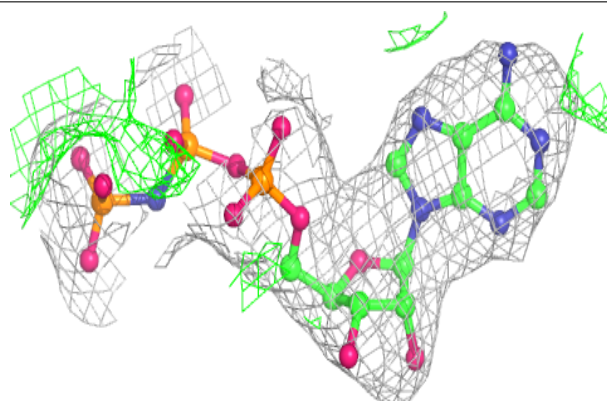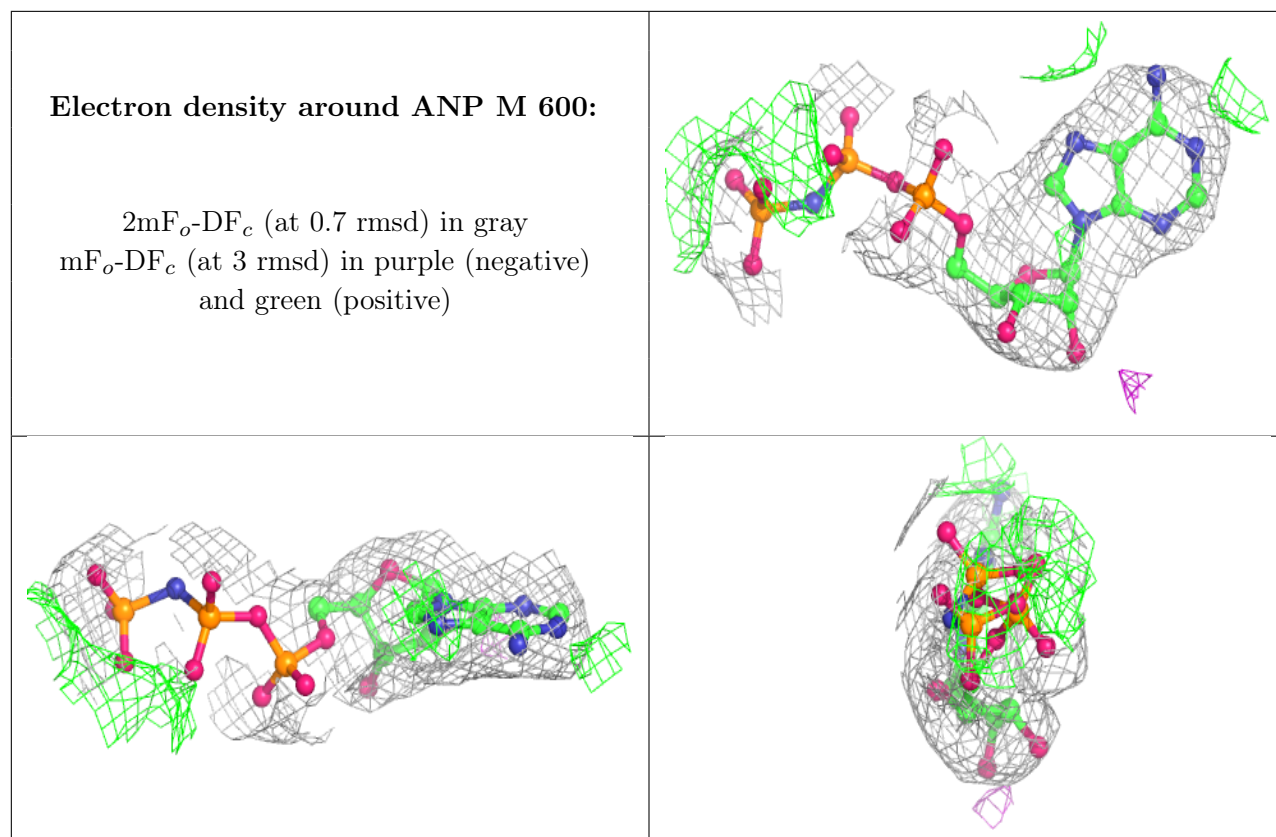and green (positive)

Electron density around ANP O 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around ANP D 600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around ANP M 600:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers (i)

There are no such residues in this entry.