wwPDB EM Validation Summary Report (i)

Dec 10, 2022 – 10:18 am GMT

PDB ID	:	5FTM
EMDB ID	:	EMD-3298
Title	:	Cryo-EM structure of human p97 bound to ATPgS (Conformation II)
Authors	:	Banerjee, S.; Bartesaghi, A.; Merk, A.; Rao, P.; Bulfer, S.L.; Yan, Y.; Green, N.; Mroczkowski, B.; Neitz, R.J.; Wipf, P.; Falconieri, V.; Deshaies, R.J.; Milne, J.L.S.; Huryn, D.; Arkin, M.; Subramaniam, S.
Deposited on	:	2016-01-14
Resolution	:	3.20 Å(reported)

This is a wwPDB EM 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/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

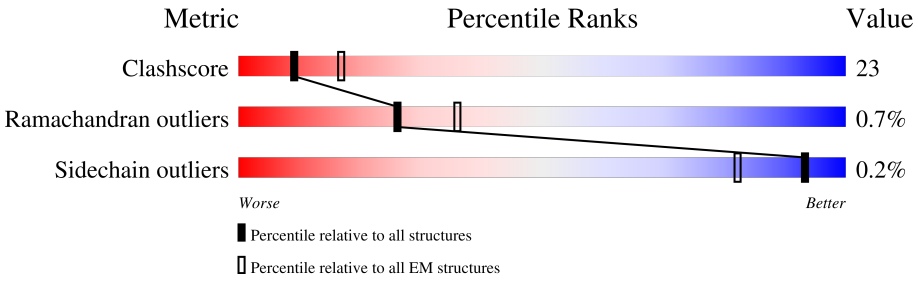
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	806	47% 52% 37% • 10%
1	B	806	47% 53% 37% • 10%
1	C	806	47% 52% 37% • 10%
1	D	806	47% 53% 37% • 10%
1	E	806	47% 53% 36% • 10%
1	F	806	47% 53% 36% • 10%

2 Entry composition (i)

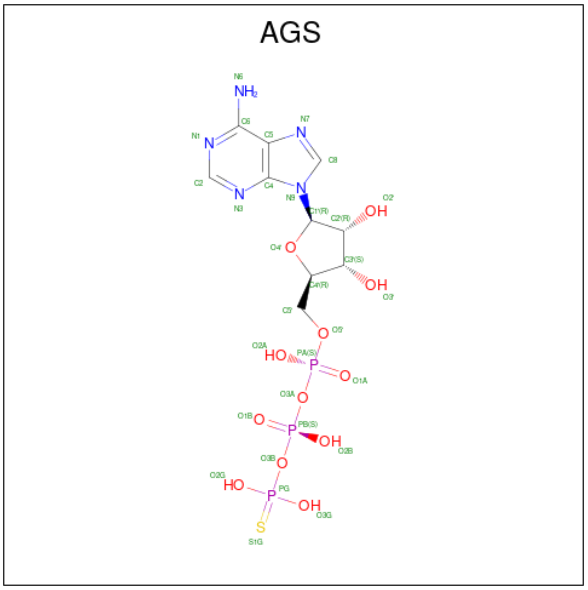
There are 4 unique types of molecules in this entry. The entry contains 34554 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE.

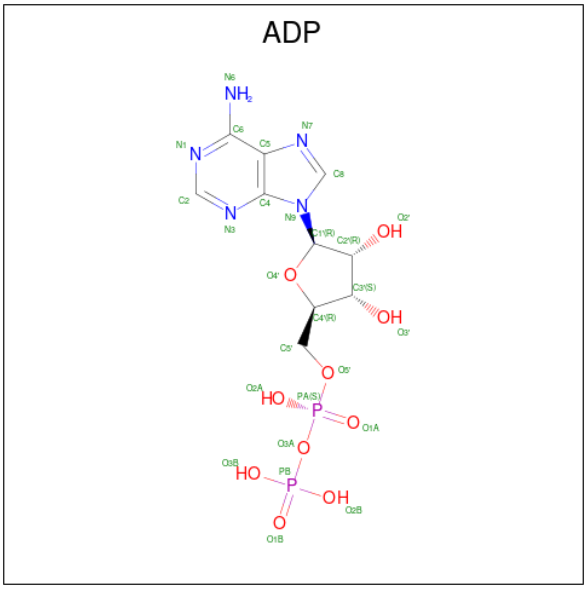
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	728	Total	C	N	O	S	0	0
			5700	3586	1005	1079	30		
1	B	728	Total	C	N	O	S	0	0
			5700	3586	1005	1079	30		
1	C	728	Total	C	N	O	S	0	0
			5700	3586	1005	1079	30		
1	D	728	Total	C	N	O	S	0	0
			5700	3586	1005	1079	30		
1	E	728	Total	C	N	O	S	0	0
			5700	3586	1005	1079	30		
1	F	728	Total	C	N	O	S	0	0
			5700	3586	1005	1079	30		

- Molecule 2 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).



Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	B	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	C	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	D	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	E	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	
2	F	1	Total	C	N	O	P	S	0
			31	10	5	12	3	1	

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

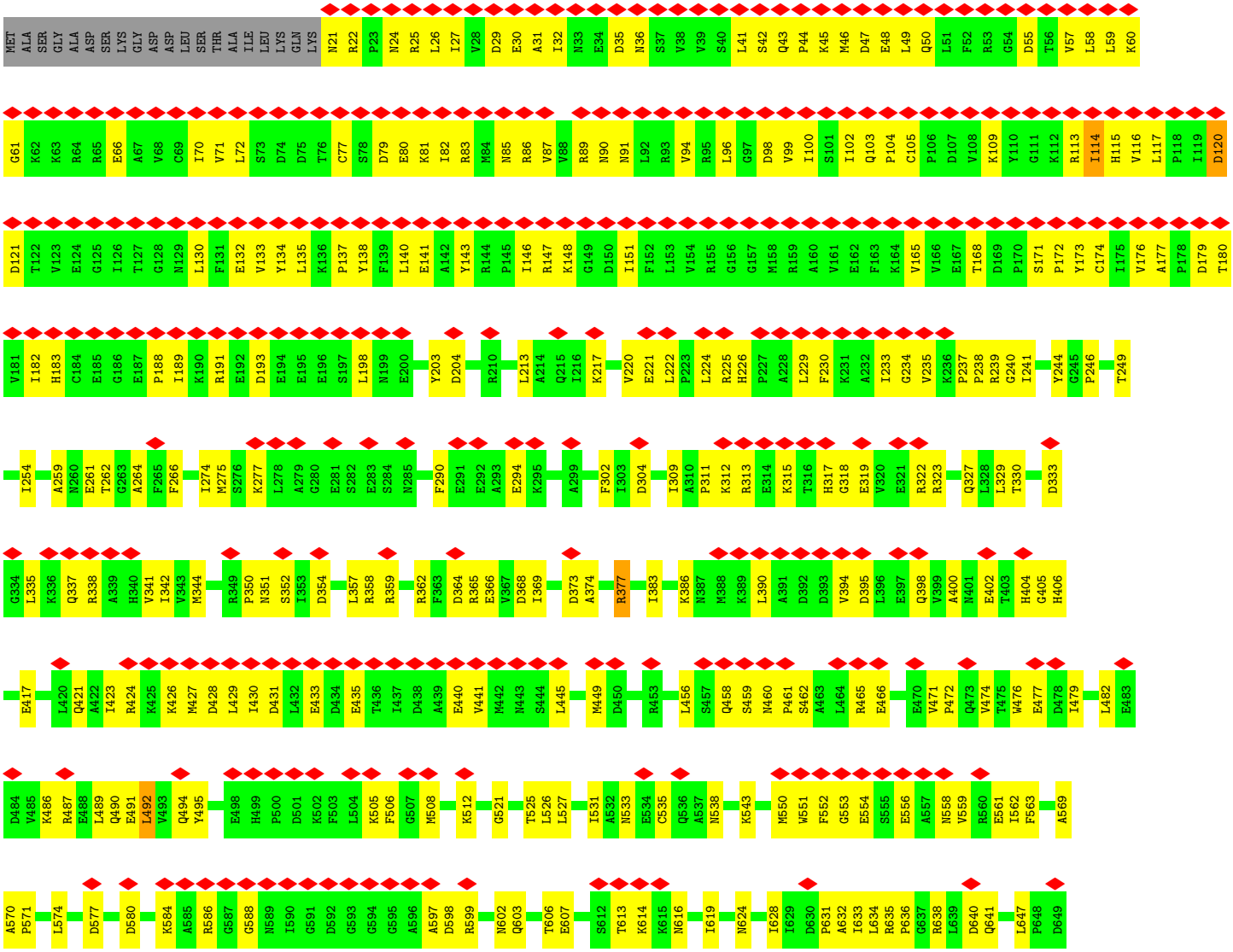
Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Mg	0
			1	1	
4	B	1	Total	Mg	0
			1	1	
4	C	1	Total	Mg	0
			1	1	
4	D	1	Total	Mg	0
			1	1	
4	E	1	Total	Mg	0
			1	1	
4	F	1	Total	Mg	0
			1	1	

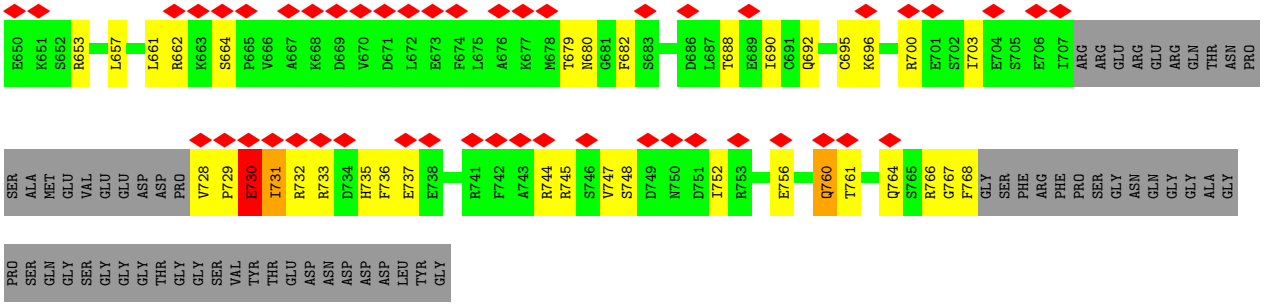
3 Residue-property plots (i)

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 atom inclusion in map 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 diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). 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: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

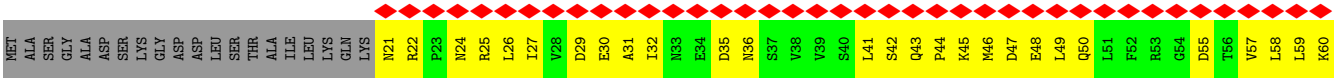
Chain A:

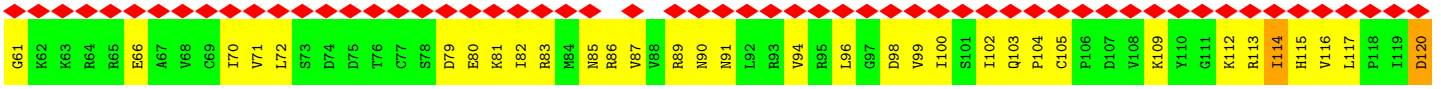


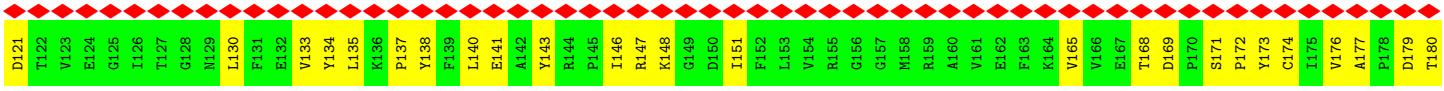


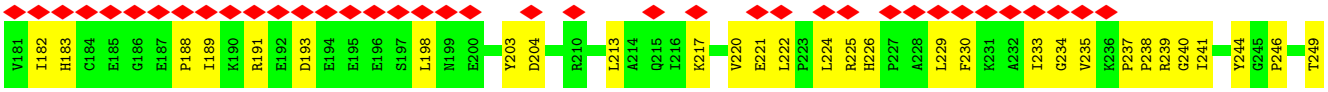
• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

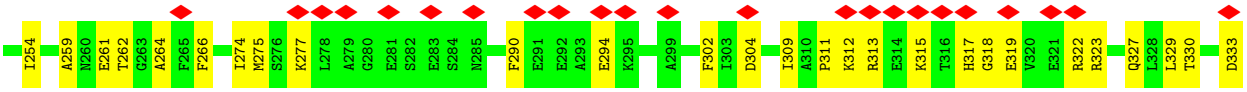
Chain B:

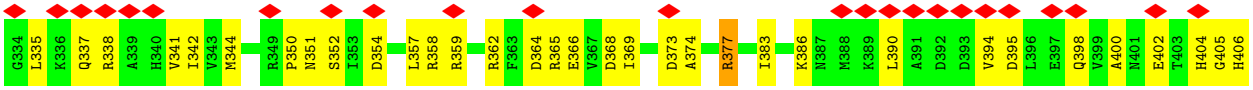


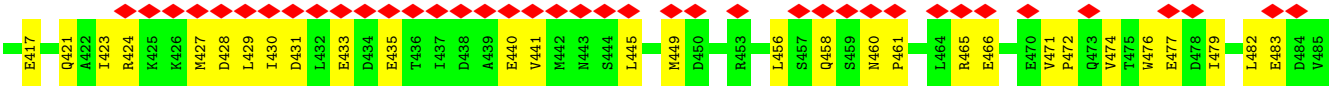


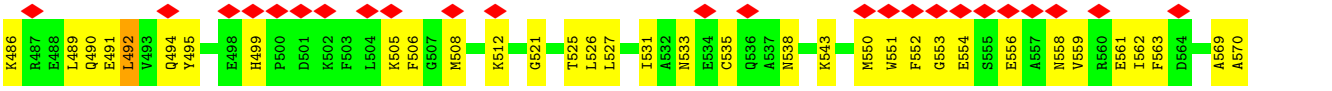


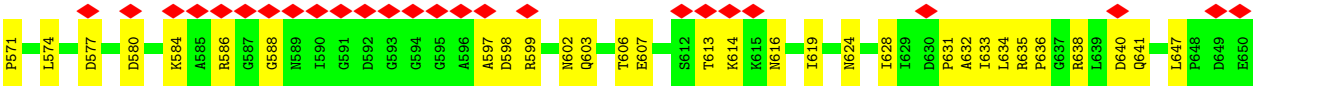


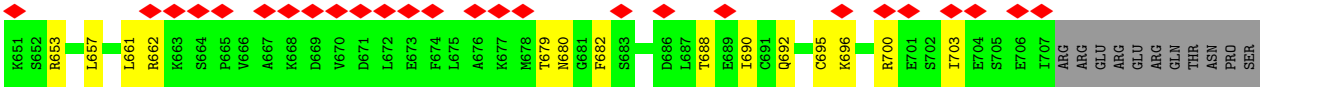


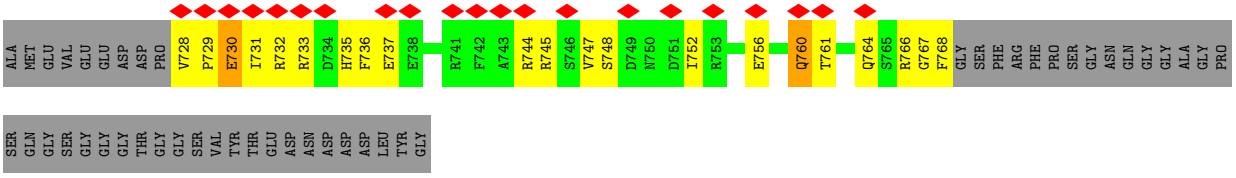






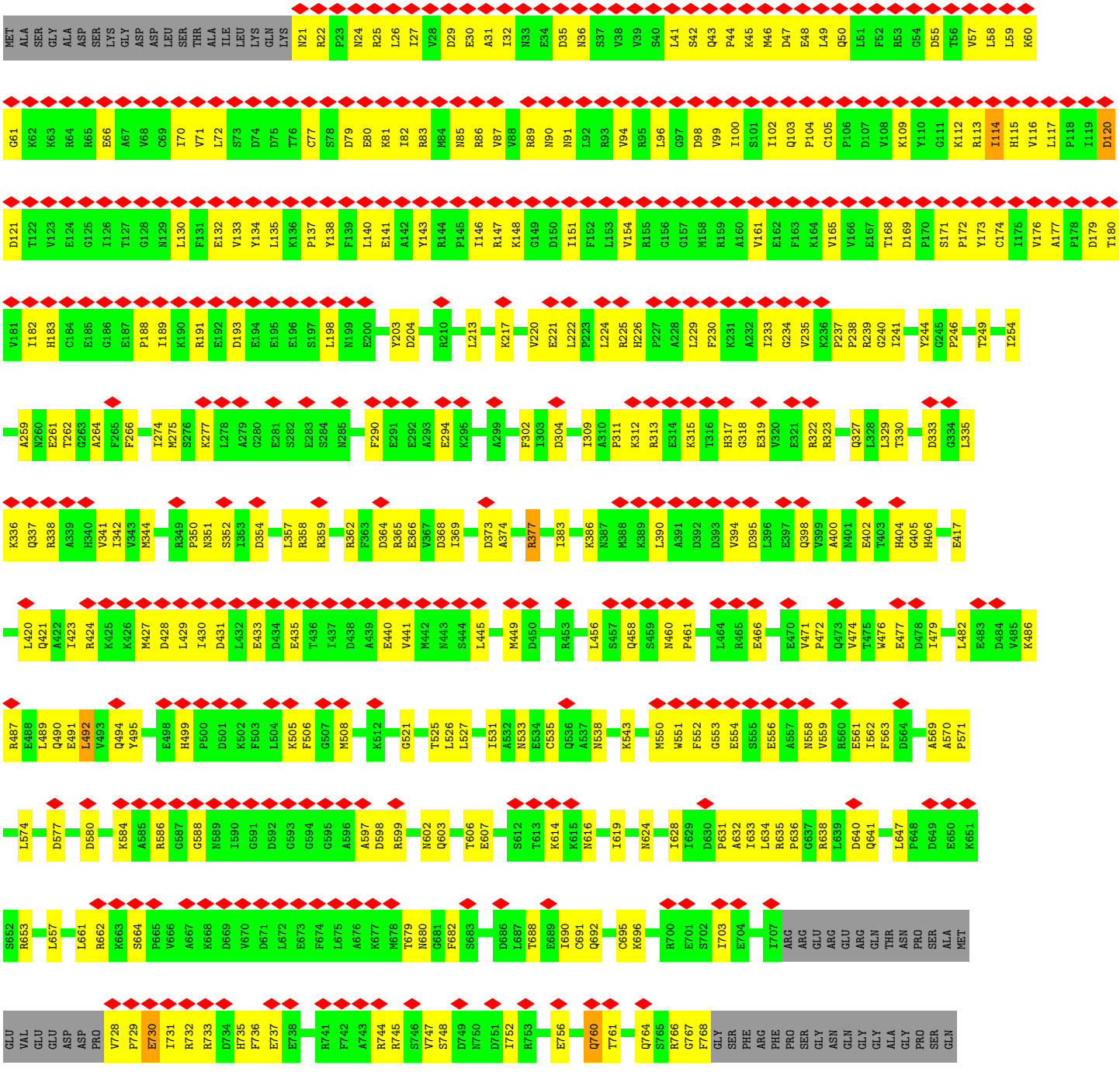






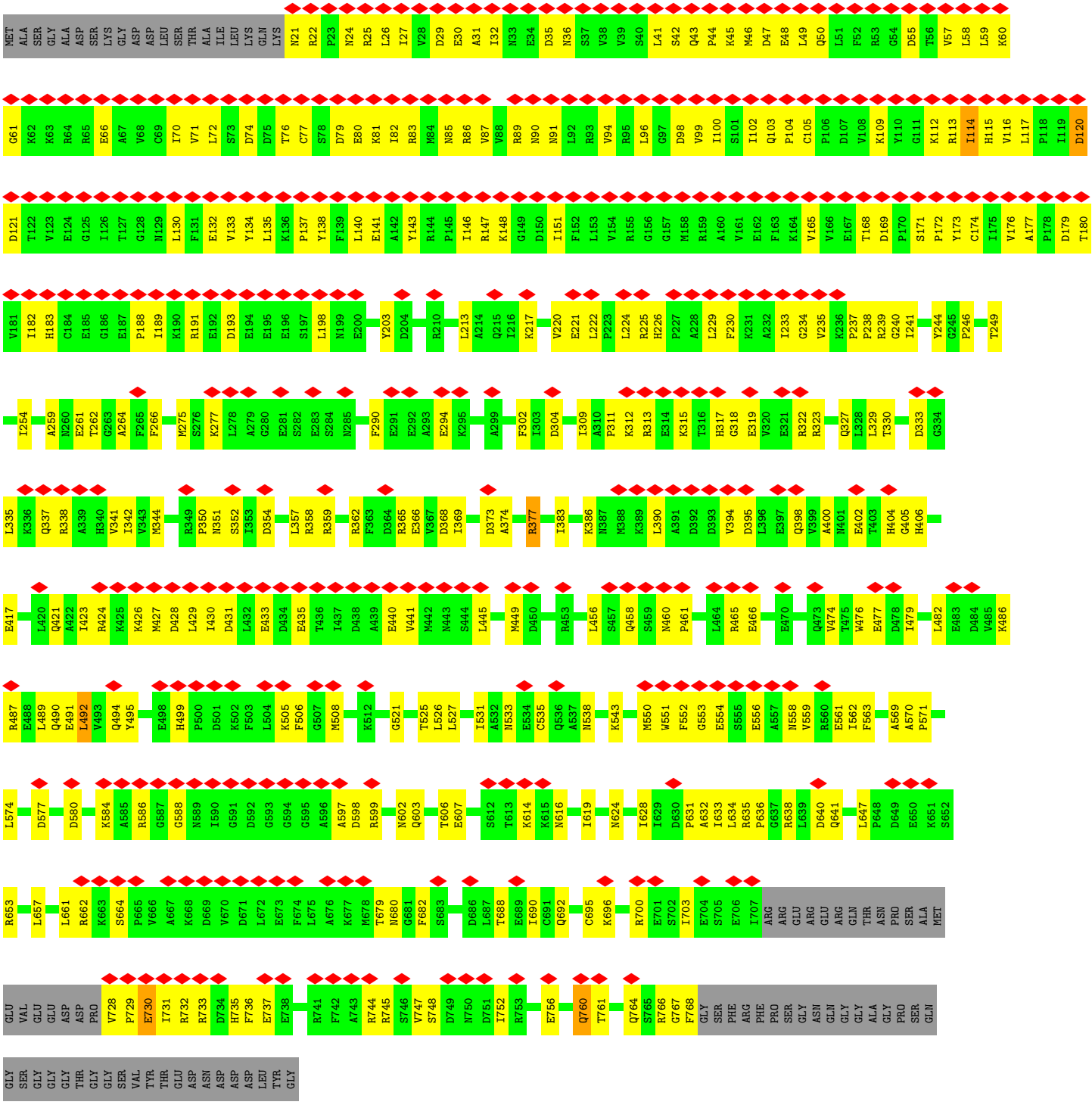
• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

Chain C:



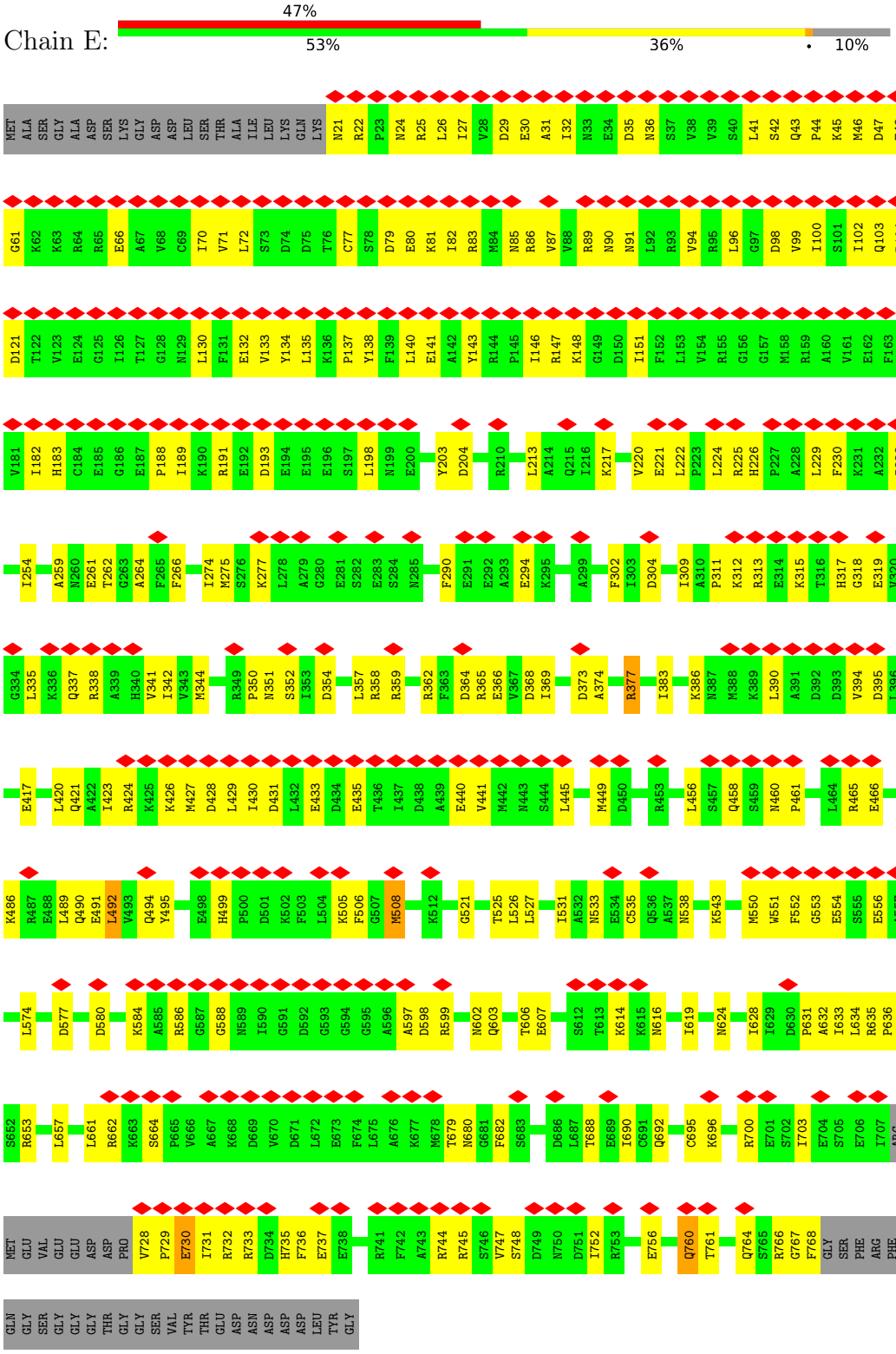
• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

Chain D:



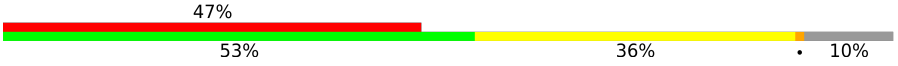
• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

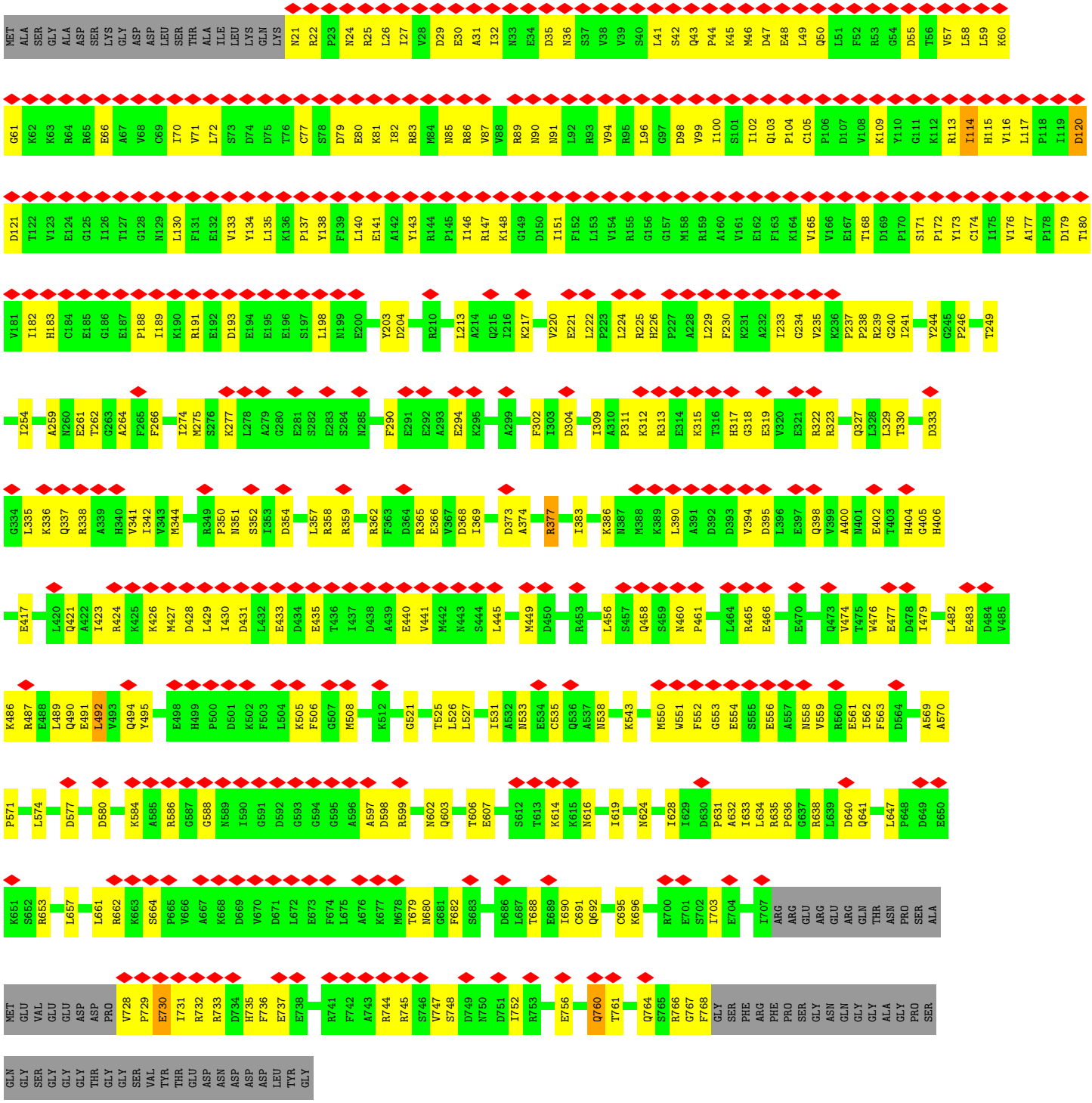
Chain E:



• Molecule 1: TRANSITIONAL ENDOPLASMIC RETICULUM ATPASE

Chain F:




MET ALA SER GLY ALA ASP SER LYS GLY ASP ASP LEU SER THR ALA ILE LEU LYS GLN LYS
N21 R22 P23 N24 R25 L26 I27 V28 D29 E30 A31 I32 N33 E34 D35 N36 S37 V38 V39 S40 L41 S42 Q43 P44 K45 M46 D47 E48 L49 Q50 L51 F52 R53 G54 D55 T56 V57 L58 L59 K60
G61 K62 K63 R64 R65 E66 A67 V68 C69 I70 V71 L72 S73 D74 D75 T76 C77 S78 D79 E80 K81 I82 R83 M84 N85 R86 V87 V88 R89 N90 N91 L92 R93 V94 R95 L96 G97 D98 V99 I100 S101 I102 Q103 P104 C105 P106 D107 V108 K109 Y110 G111 K112 R113 I114 H115 V116 L117 P118 I119 D120
D121 T122 V123 E124 G125 I126 T127 G128 N129 L130 F131 E132 V133 Y134 L135 K136 P137 Y138 F139 L140 E141 A142 Y143 R144 P145 I146 R147 K148 G149 D150 I151 F152 L153 V154 R155 G156 G157 M158 R159 A160 V161 E162 F163 K164 V165 V166 E167 T168 D169 P170 S171 P172 Y173 C174 I175 V176 A177 P178 D179 T180
V181 I182 H183 C184 E185 G186 E187 P188 I189 K190 R191 E192 D193 E194 E195 E196 S197 L198 N199 E200 Y203 D204 R210 L213 A214 Q215 I216 K217 V220 E221 L222 P223 L224 R225 H226 P227 A228 L229 F230 K231 A232 I233 G234 V235 K236 P237 P238 R239 G240 I241 Y244 G245 P246 T249
I254 A259 N260 E261 T262 G263 A264 F265 F266 I274 M275 S276 K277 L278 A279 G280 E281 S282 E283 S284 N285 F290 E291 E292 A293 E294 K295 A299 F302 I303 D304 I309 A310 P311 K312 R313 E314 K315 T316 H317 G318 E319 V320 E321 R322 R323 Q327 L328 L329 T330 D333
G334 L335 K336 Q337 R338 A339 H340 V341 I342 V343 M344 R349 P350 N351 S352 I353 D354 L357 R358 R359 R362 F363 D364 R365 E366 V367 D368 I369 D373 A374 R377 I383 K386 N387 M388 K389 L390 A391 D392 D393 V394 D395 L396 E397 Q398 V399 A400 N401 E402 T403 H404 G405 H406
E417 L420 Q421 A422 I423 R424 K425 K426 M427 D428 L429 I430 D431 L432 E433 D434 E435 T436 I437 D438 A439 E440 V441 M442 N443 S444 L445 M449 D450 R453 L456 S457 Q458 S459 N460 P461 L464 R465 E466 E470 Q473 V474 T475 W476 E477 D478 I479 L482 E483 D484 V485
K486 R487 E488 L489 Q490 E491 L492 V493 Q494 Y495 E498 H499 P500 D501 K502 F503 L504 K505 F506 G507 M508 K512 G621 T525 L526 L527 I631 A532 N533 E534 C535 Q536 A537 N538 K643 M550 W551 F552 G553 E554 S555 E556 A557 N558 V559 R560 E561 I562 F563 D564 A569 A570
P571 L574 D577 D580 K584 A585 R586 G587 G588 N589 I590 G591 D592 G593 G594 G595 A596 A597 D598 R599 N602 Q603 T606 E607 S612 T613 K614 K615 N616 I619 N624 I628 I629 D630 P631 A632 I633 L634 R635 P636 G637 R638 L639 D640 Q641 L647 P648 D649 E650
K651 S652 R653 L657 L661 R662 K663 S664 P665 V666 A667 K668 D669 V670 D671 L672 E673 F674 L675 A676 K677 M678 T679 N680 G681 F682 S683 D686 L687 T688 E689 I690 C691 Q692 C695 K696 R700 E701 S702 I703 E704 I707 ARG ARG GLU ARG GLU GLN THR ASN PRO SER ALA
MET GLU VAL GLU GLU ASP ASP PRO V728 P729 E730 I731 R732 R733 D734 H735 F736 E737 E738 R741 F742 A743 R744 R745 S746 V747 S748 D749 N750 D751 I752 R753 E756 Q760 T761 Q764 S765 R766 G767 F768 GLY SER PHE ARG PHE PRO SER GLY ASN GLN GLY GLY ALA GLY PRO SER
GLN GLY SER GLY GLY GLY THR GLY GLY SER VAL TYR THR GLU ASP ASN ASP ASP ASP LEU TYR GLY

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C6	Depositor
Number of particles used	32406	Depositor
Resolution determination method	Not provided	
CTF correction method	EACH PARTICLE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	950	Depositor
Maximum defocus (nm)	2700	Depositor
Magnification	36980	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.071	Depositor
Minimum map value	-0.025	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0183	Depositor
Map size (Å)	186.576, 186.576, 186.576	wwPDB
Map dimensions	276, 276, 276	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.676, 0.676, 0.676	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, AGS, 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	0.59	0/5793	0.69	3/7822 (0.0%)
1	B	0.59	0/5793	0.68	1/7822 (0.0%)
1	C	0.59	0/5793	0.68	1/7822 (0.0%)
1	D	0.59	0/5793	0.68	1/7822 (0.0%)
1	E	0.59	0/5793	0.68	1/7822 (0.0%)
1	F	0.59	0/5793	0.68	1/7822 (0.0%)
All	All	0.59	0/34758	0.68	8/46932 (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	A	0	2
1	B	0	2
1	C	0	2
1	D	0	2
1	E	0	2
1	F	0	2
All	All	0	12

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	730	GLU	CB-CA-C	7.15	124.70	110.40
1	A	731	ILE	N-CA-C	-6.49	93.49	111.00
1	C	104	PRO	C-N-CA	-5.82	107.14	121.70
1	B	104	PRO	C-N-CA	-5.82	107.15	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	104	PRO	C-N-CA	-5.82	107.16	121.70

There are no chirality outliers.

5 of 12 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	359	ARG	Sidechain
1	A	377	ARG	Sidechain
1	B	359	ARG	Sidechain
1	B	377	ARG	Sidechain
1	C	359	ARG	Sidechain

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	5700	0	5769	285	0
1	B	5700	0	5769	285	0
1	C	5700	0	5769	287	0
1	D	5700	0	5769	285	0
1	E	5700	0	5769	288	0
1	F	5700	0	5769	288	0
2	A	31	0	12	6	0
2	B	31	0	12	6	0
2	C	31	0	12	6	0
2	D	31	0	12	6	0
2	E	31	0	12	6	0
2	F	31	0	12	6	0
3	A	27	0	12	0	0
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
3	E	27	0	12	0	0
3	F	27	0	12	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
All	All	34554	0	34758	1584	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 23.

The worst 5 of 1584 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:E:312:LYS:HD3	1:E:315:LYS:HD3	1.29	1.15
1:F:312:LYS:HD3	1:F:315:LYS:HD3	1.29	1.15
1:D:312:LYS:HD3	1:D:315:LYS:HD3	1.29	1.12
1:A:312:LYS:HD3	1:A:315:LYS:HD3	1.29	1.12
1:C:312:LYS:HD2	1:C:315:LYS:HB2	1.32	1.11

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 PDB entries followed by that with respect to all EM entries.

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	724/806 (90%)	664 (92%)	55 (8%)	5 (1%)	22	61
1	B	724/806 (90%)	664 (92%)	55 (8%)	5 (1%)	22	61
1	C	724/806 (90%)	664 (92%)	55 (8%)	5 (1%)	22	61
1	D	724/806 (90%)	664 (92%)	55 (8%)	5 (1%)	22	61
1	E	724/806 (90%)	664 (92%)	54 (8%)	6 (1%)	19	58
1	F	724/806 (90%)	664 (92%)	55 (8%)	5 (1%)	22	61
All	All	4344/4836 (90%)	3984 (92%)	329 (8%)	31 (1%)	26	61

5 of 31 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	730	GLU
1	C	730	GLU
1	D	730	GLU
1	E	730	GLU
1	F	730	GLU

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 PDB entries followed by that with respect to all EM entries.

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	619/678 (91%)	618 (100%)	1 (0%)	93	98
1	B	619/678 (91%)	618 (100%)	1 (0%)	93	98
1	C	619/678 (91%)	618 (100%)	1 (0%)	93	98
1	D	619/678 (91%)	618 (100%)	1 (0%)	93	98
1	E	619/678 (91%)	618 (100%)	1 (0%)	93	98
1	F	619/678 (91%)	618 (100%)	1 (0%)	93	98
All	All	3714/4068 (91%)	3708 (100%)	6 (0%)	93	98

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	492	LEU
1	E	492	LEU
1	F	492	LEU
1	B	492	LEU
1	A	492	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 49 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	533	ASN
1	E	499	HIS

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Mol	Chain	Res	Type
1	D	538	ASN
1	E	36	ASN
1	E	538	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 6 are monoatomic - leaving 12 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	$\#\|Z\| > 2$
3	ADP	A	902	-	24,29,29	1.09	1 (4%)	29,45,45	1.54	5 (17%)
2	AGS	C	901	4	26,33,33	1.87	3 (11%)	26,52,52	1.58	4 (15%)
2	AGS	D	901	4	26,33,33	1.87	3 (11%)	26,52,52	1.59	4 (15%)
3	ADP	C	902	-	24,29,29	1.09	1 (4%)	29,45,45	1.55	5 (17%)
3	ADP	F	902	-	24,29,29	1.08	1 (4%)	29,45,45	1.54	5 (17%)
2	AGS	E	901	4	26,33,33	1.87	3 (11%)	26,52,52	1.59	4 (15%)
3	ADP	D	902	-	24,29,29	1.09	1 (4%)	29,45,45	1.54	5 (17%)
2	AGS	B	901	4	26,33,33	1.87	3 (11%)	26,52,52	1.58	4 (15%)
2	AGS	A	901	4	26,33,33	1.87	3 (11%)	26,52,52	1.59	4 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	AGS	F	901	4	26,33,33	1.87	3 (11%)	26,52,52	1.58	4 (15%)
3	ADP	B	902	-	24,29,29	1.09	1 (4%)	29,45,45	1.54	5 (17%)
3	ADP	E	902	-	24,29,29	1.09	1 (4%)	29,45,45	1.54	5 (17%)

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
3	ADP	A	902	-	-	4/12/32/32	0/3/3/3
2	AGS	C	901	4	-	6/17/38/38	0/3/3/3
2	AGS	D	901	4	-	6/17/38/38	0/3/3/3
3	ADP	C	902	-	-	4/12/32/32	0/3/3/3
3	ADP	F	902	-	-	4/12/32/32	0/3/3/3
2	AGS	E	901	4	-	6/17/38/38	0/3/3/3
3	ADP	D	902	-	-	4/12/32/32	0/3/3/3
2	AGS	B	901	4	-	6/17/38/38	0/3/3/3
2	AGS	A	901	4	-	6/17/38/38	0/3/3/3
2	AGS	F	901	4	-	6/17/38/38	0/3/3/3
3	ADP	B	902	-	-	4/12/32/32	0/3/3/3
3	ADP	E	902	-	-	4/12/32/32	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	901	AGS	PG-S1G	7.86	2.07	1.90
2	A	901	AGS	PG-S1G	7.86	2.07	1.90
2	D	901	AGS	PG-S1G	7.86	2.07	1.90
2	B	901	AGS	PG-S1G	7.85	2.07	1.90
2	E	901	AGS	PG-S1G	7.85	2.07	1.90

The worst 5 of 54 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	901	AGS	PA-O3A-PB	-3.57	120.57	132.83
2	F	901	AGS	PA-O3A-PB	-3.57	120.57	132.83
2	A	901	AGS	PA-O3A-PB	-3.56	120.60	132.83
2	B	901	AGS	PA-O3A-PB	-3.56	120.62	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	901	AGS	PA-O3A-PB	-3.56	120.62	132.83

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	AGS	O4'-C4'-C5'-O5'
2	A	901	AGS	C3'-C4'-C5'-O5'
2	B	901	AGS	O4'-C4'-C5'-O5'
2	B	901	AGS	C3'-C4'-C5'-O5'
2	C	901	AGS	O4'-C4'-C5'-O5'

There are no ring outliers.

6 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	901	AGS	6	0
2	D	901	AGS	6	0
2	E	901	AGS	6	0
2	B	901	AGS	6	0
2	A	901	AGS	6	0
2	F	901	AGS	6	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.

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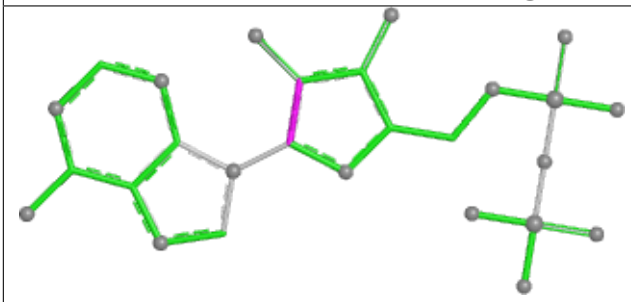
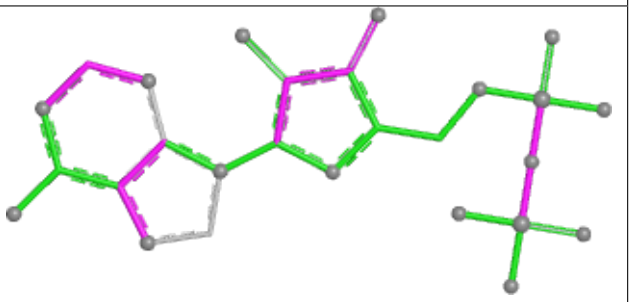
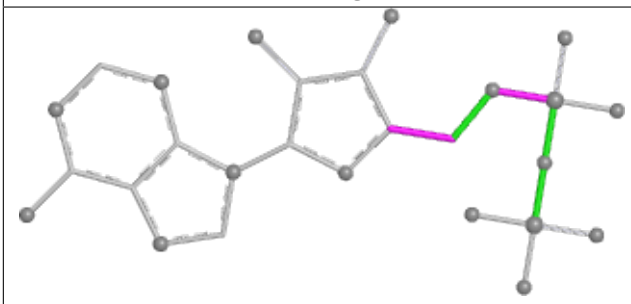
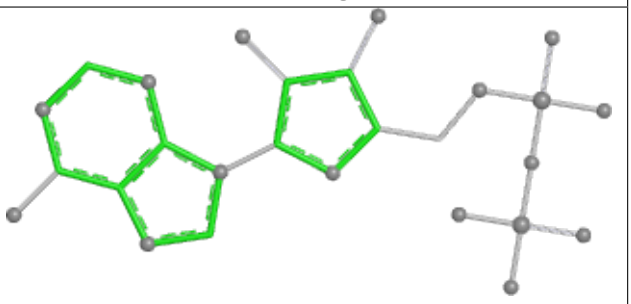
 Bond lengths	 Bond angles
 Torsions	 Rings

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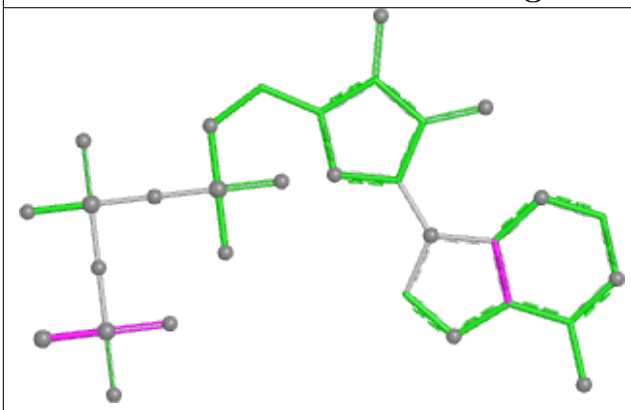
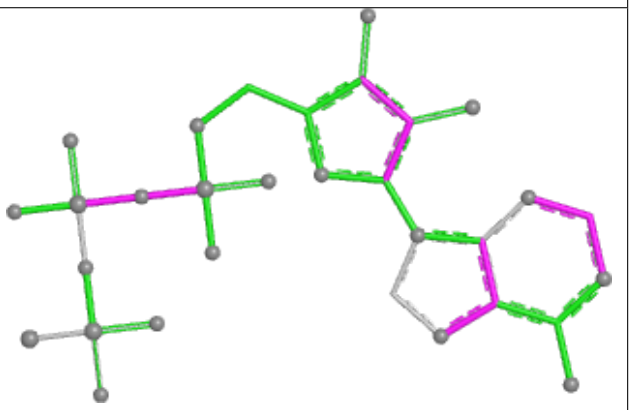
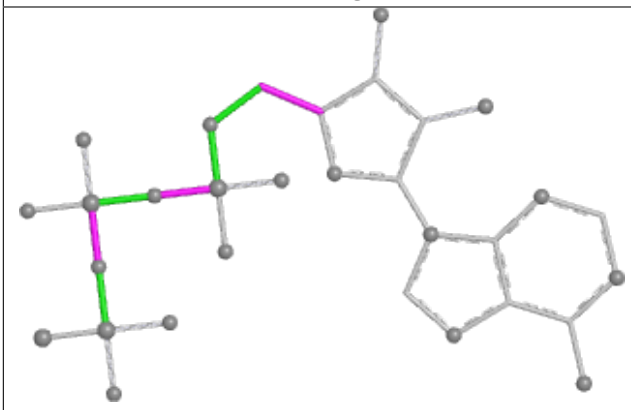
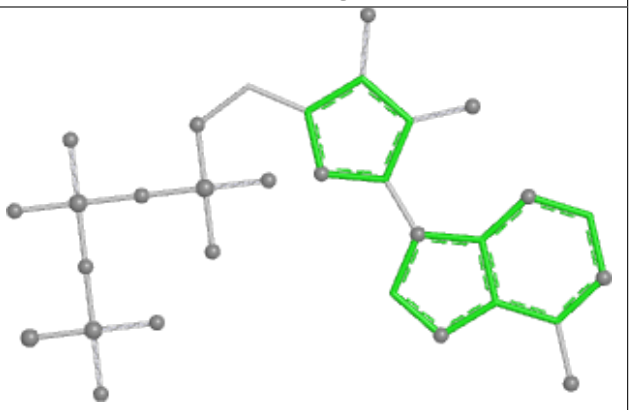
 Bond lengths	 Bond angles
 Torsions	 Rings

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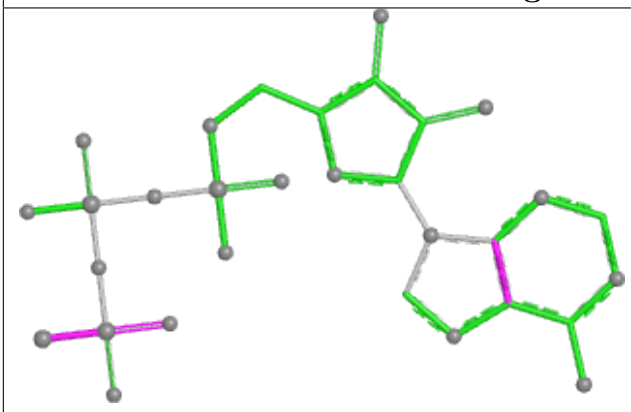
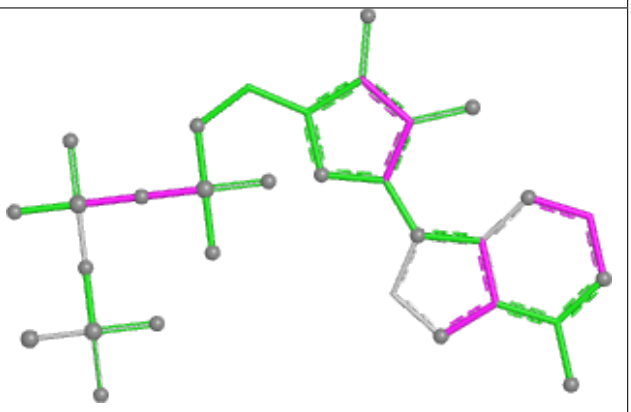
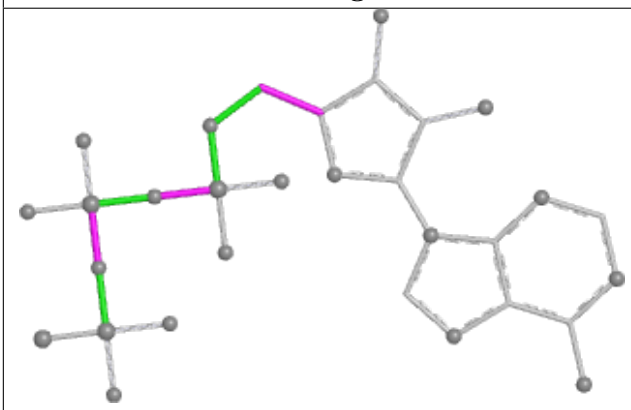
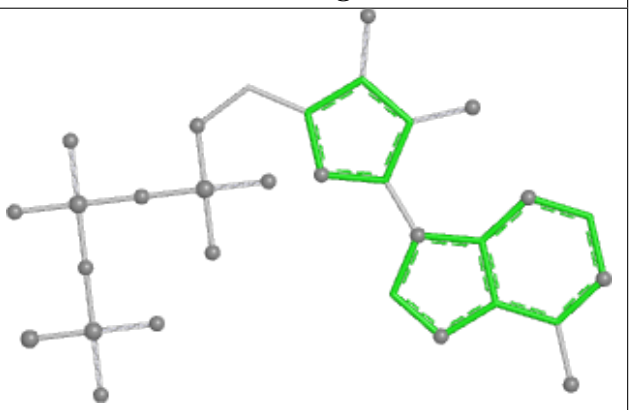
 Bond lengths	 Bond angles
 Torsions	 Rings

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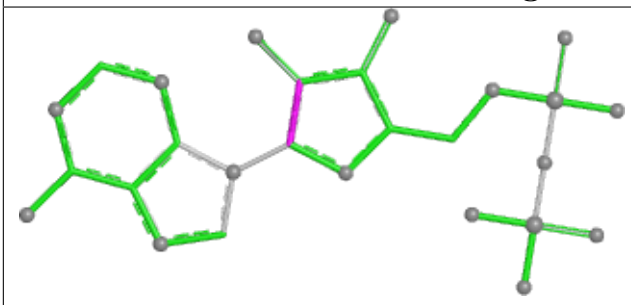
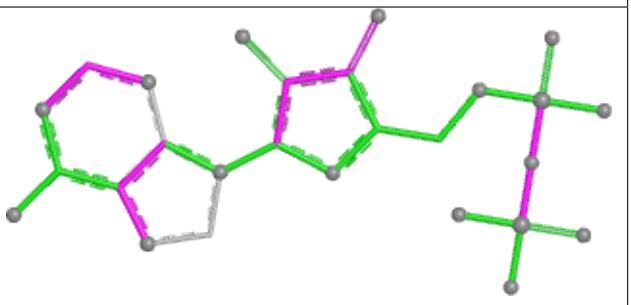
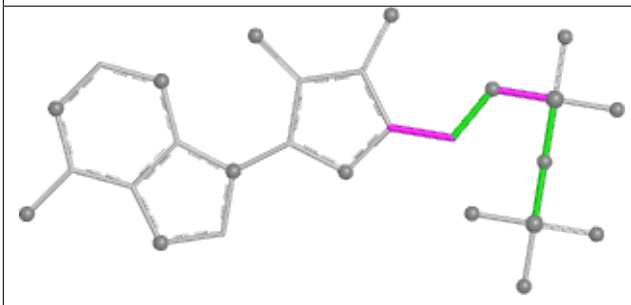
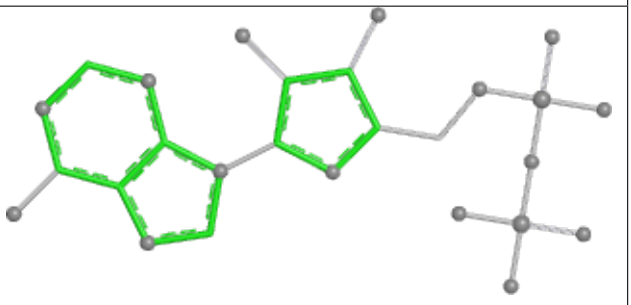
 Bond lengths	 Bond angles
 Torsions	 Rings

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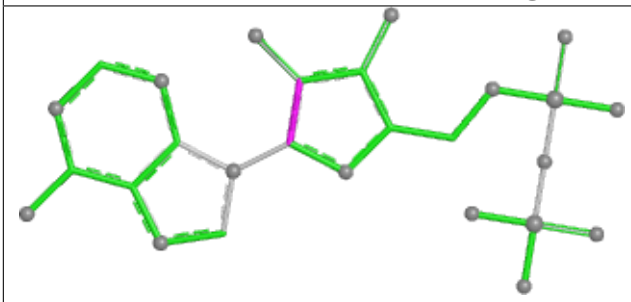
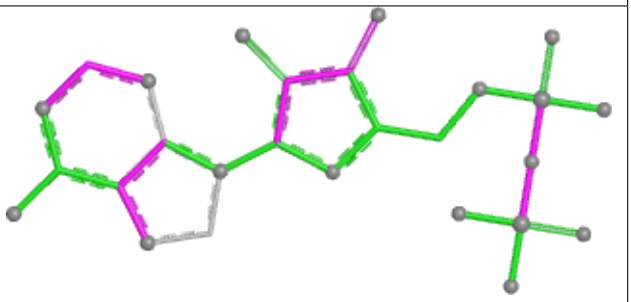
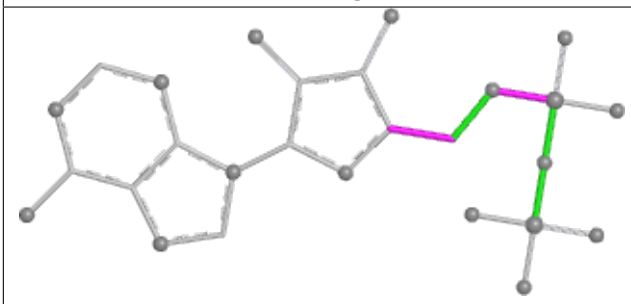
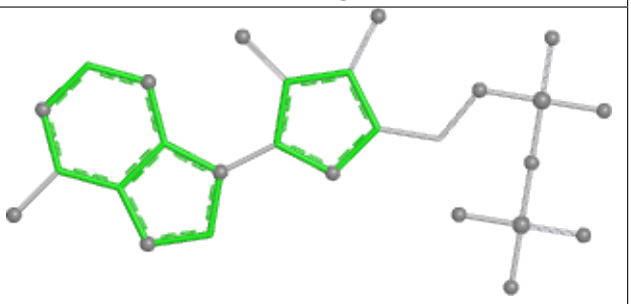
 Bond lengths	 Bond angles
 Torsions	 Rings

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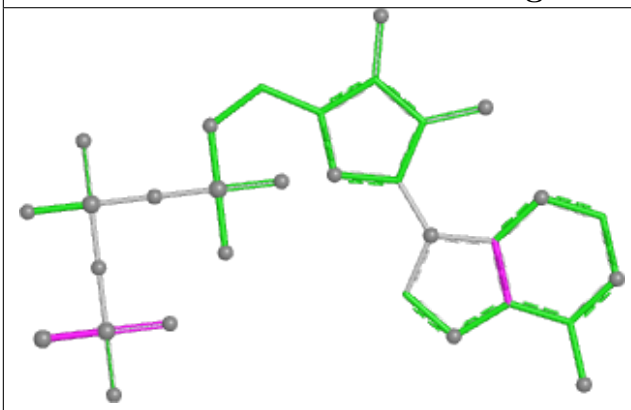
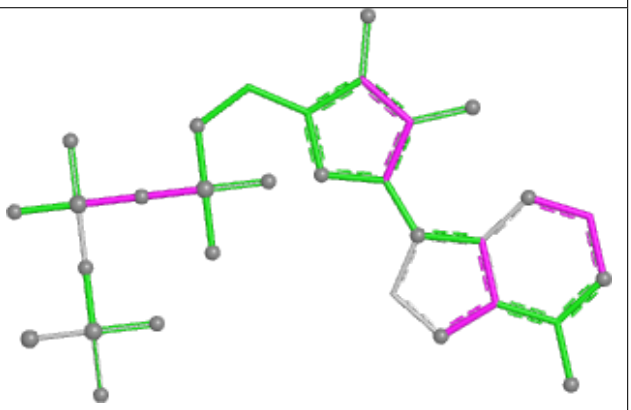
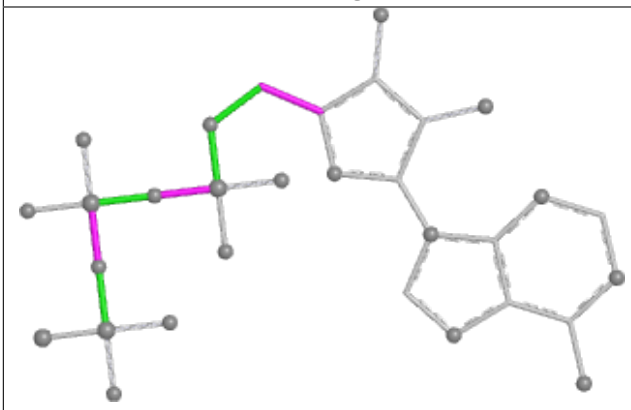
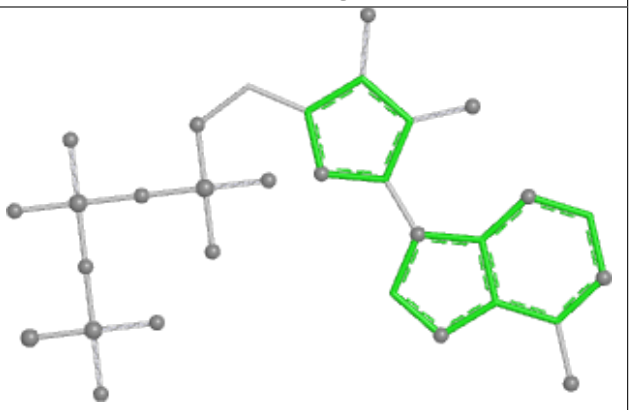
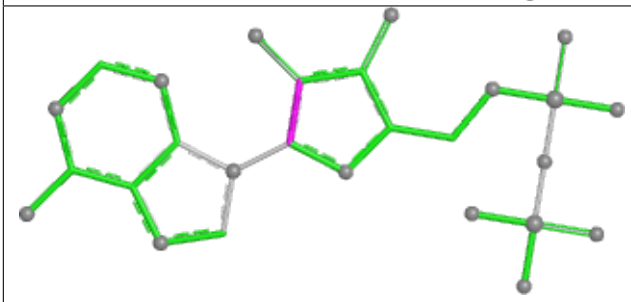
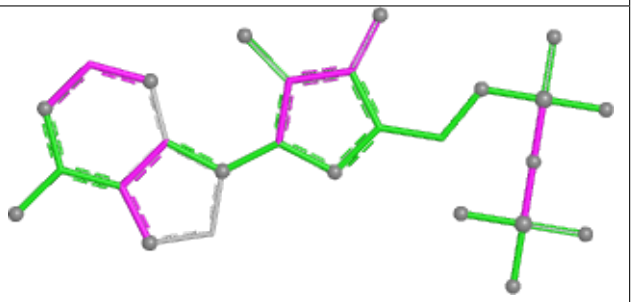
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP D 902



Bond lengths



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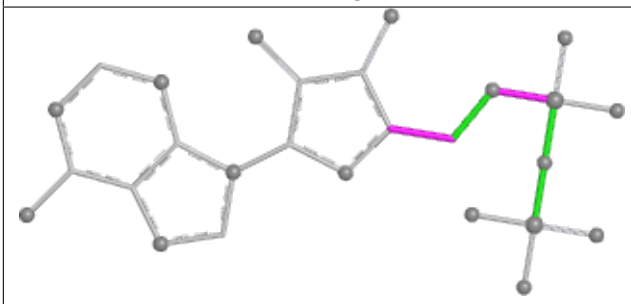

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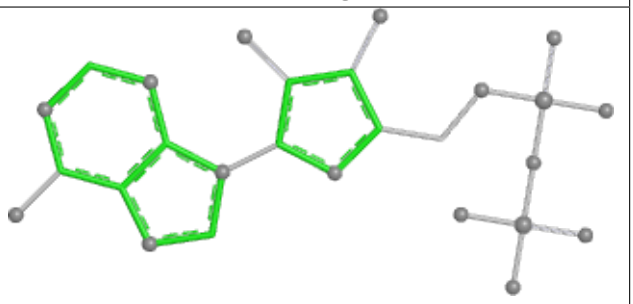
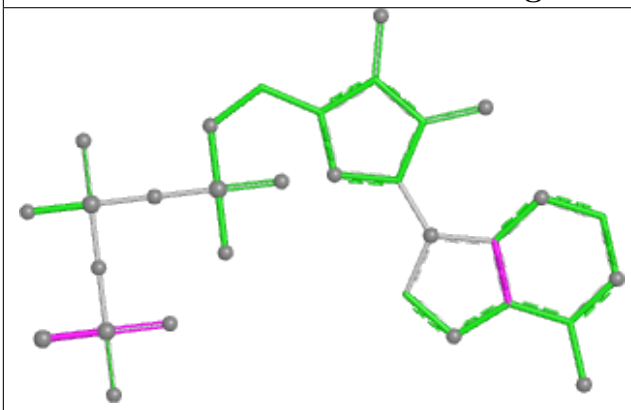


Rings

Ligand AGS B 901



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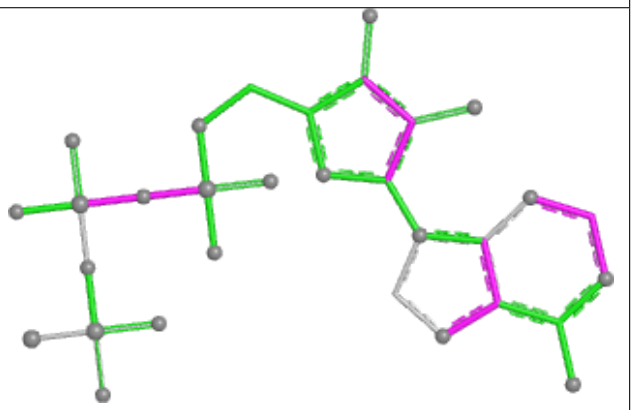

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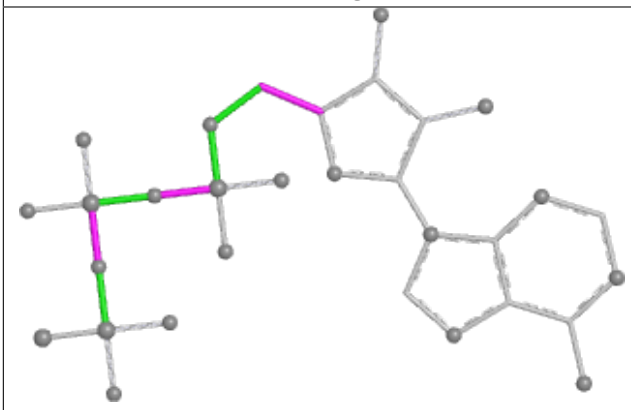
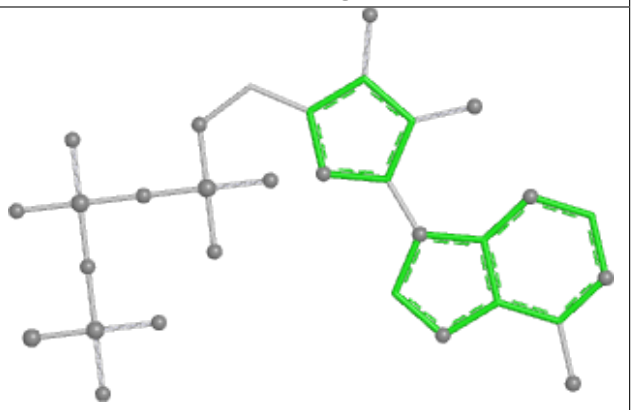
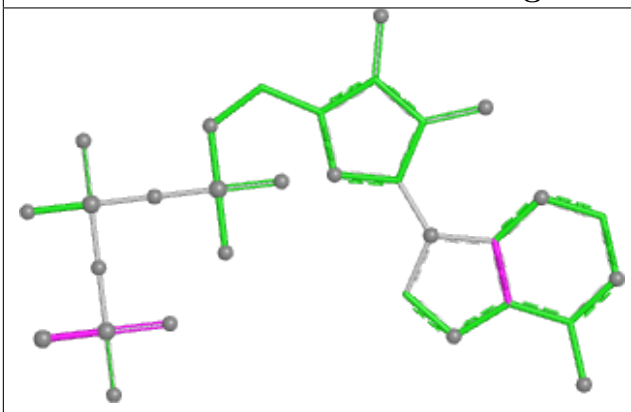


Torsions

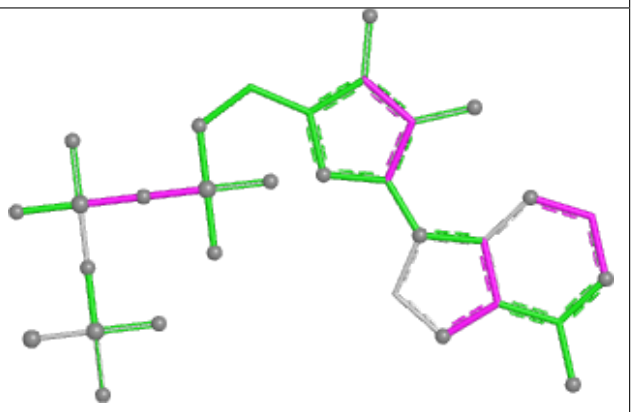


Rings

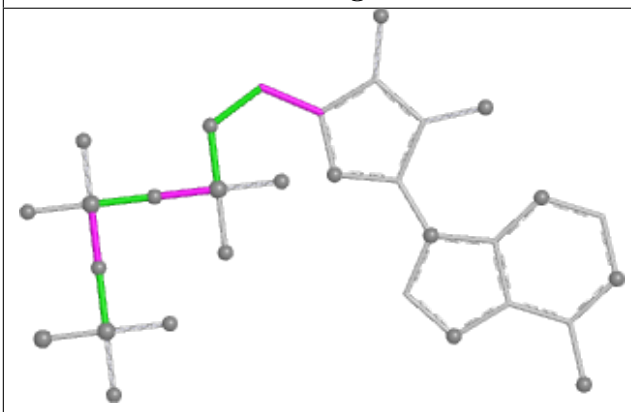
Ligand AGS A 901



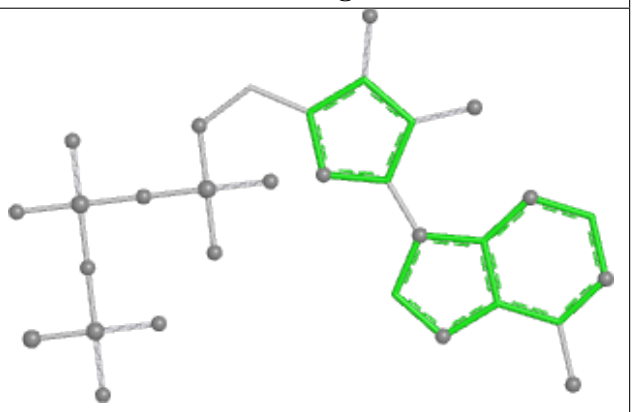
Bond lengths



Bond angles

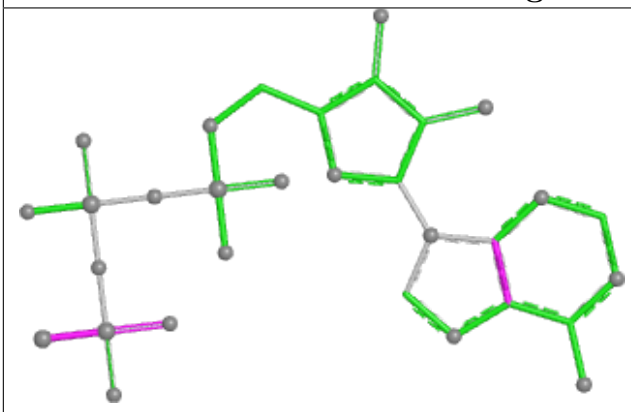


Torsions

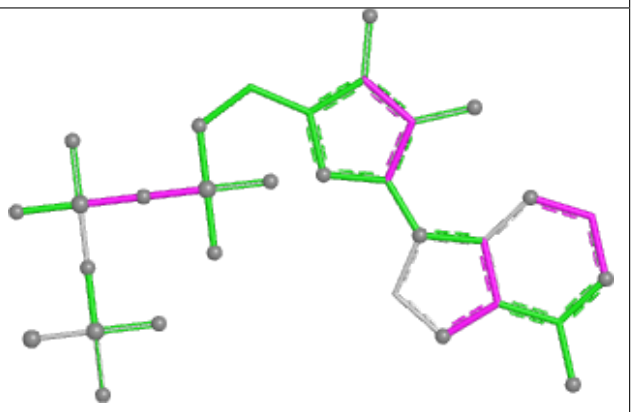


Rings

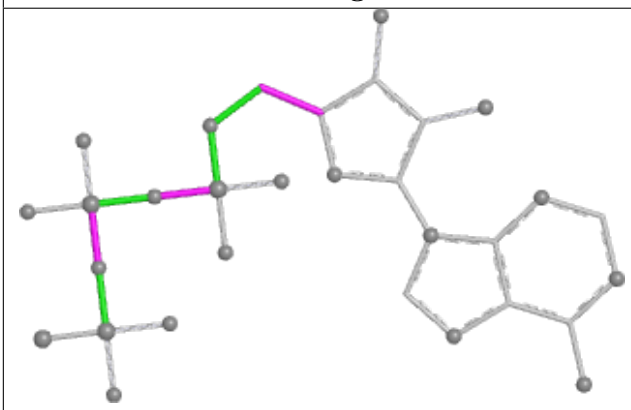
Ligand AGS F 901



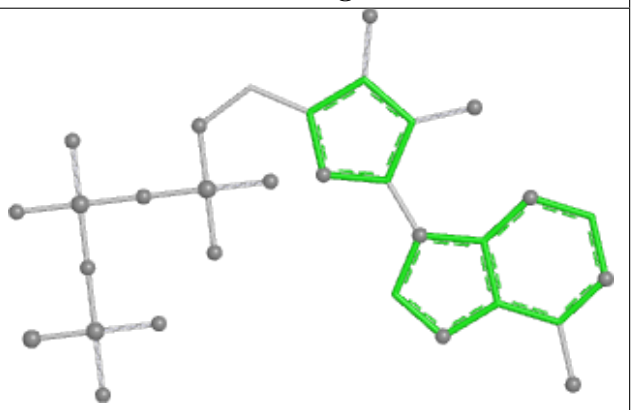
Bond lengths



Bond angles

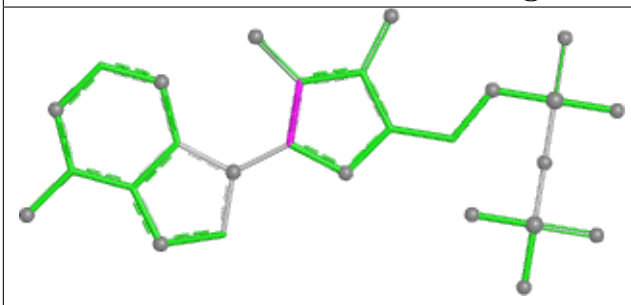


Torsions

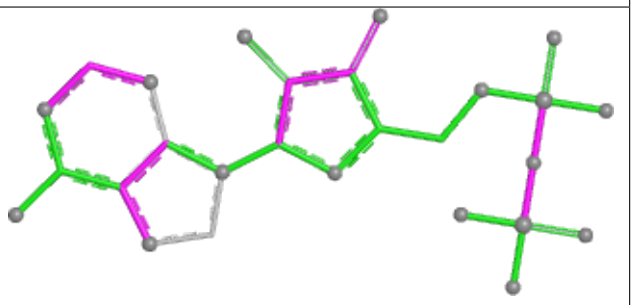


Rings

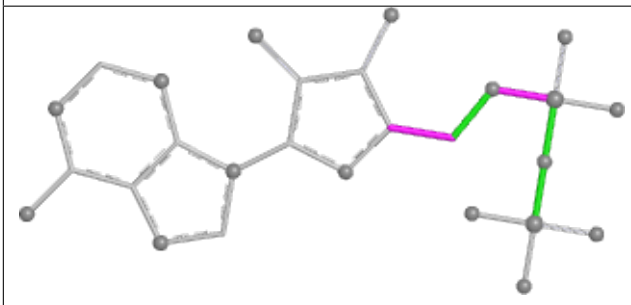
Ligand ADP B 902



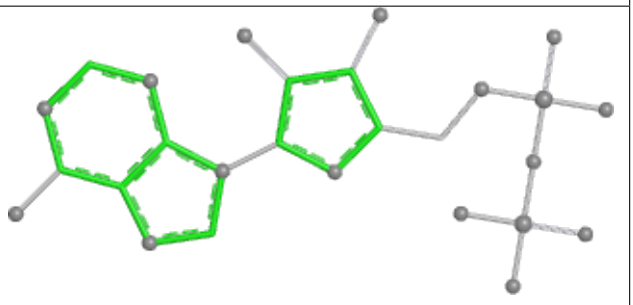
Bond lengths



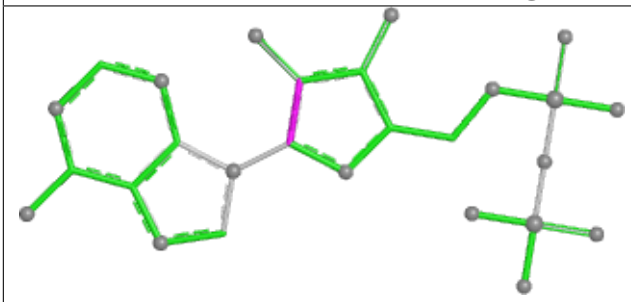
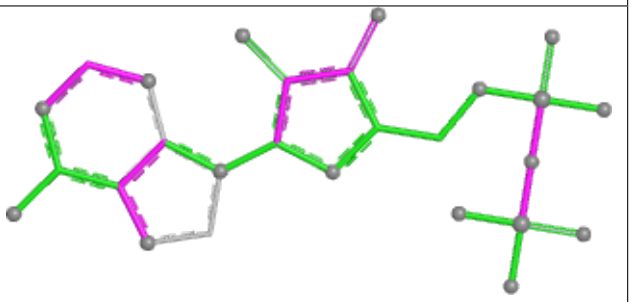
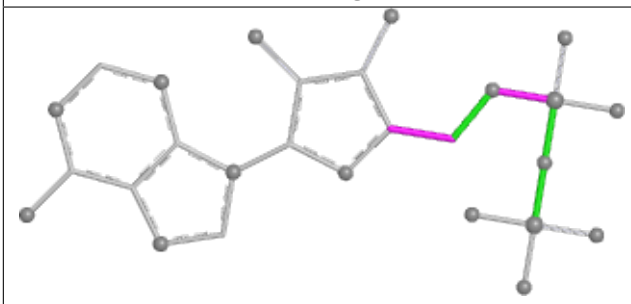
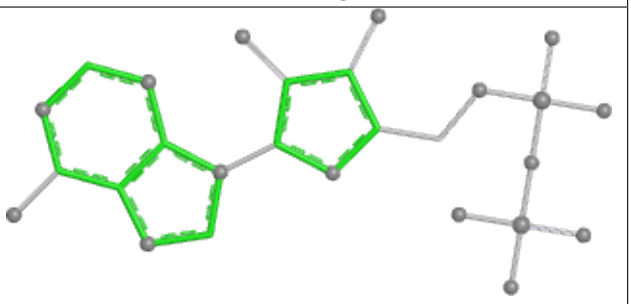
Bond angles



Torsions



Rings

Ligand ADP E 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

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.

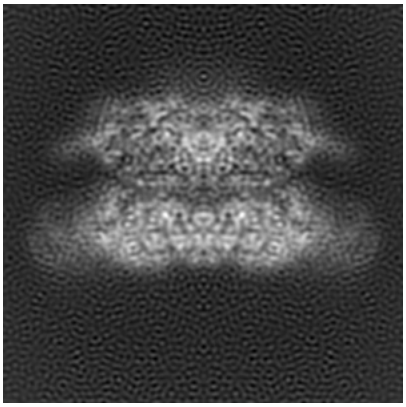
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3298. These allow visual inspection of the internal detail of the map and identification of artifacts.

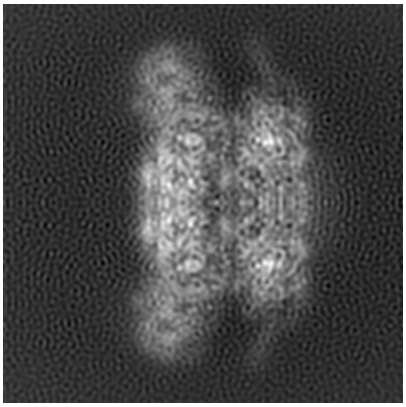
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

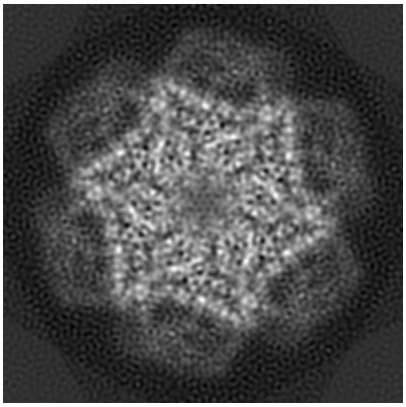
6.1.1 Primary map



X



Y

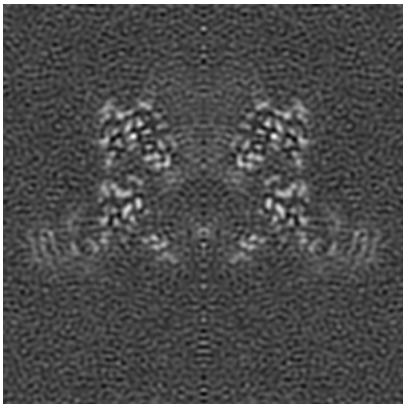


Z

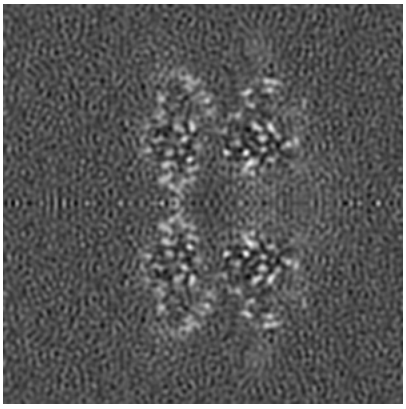
The images above show the map projected in three orthogonal directions.

6.2 Central slices

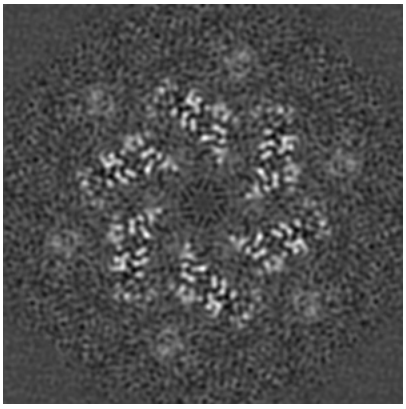
6.2.1 Primary map



X Index: 138



Y Index: 138

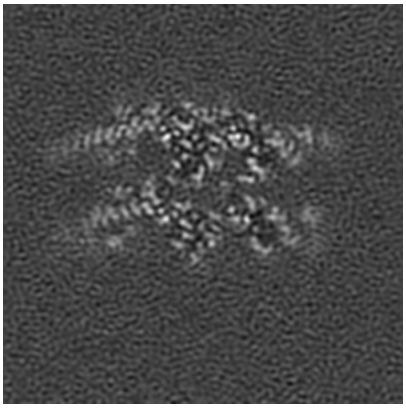


Z Index: 138

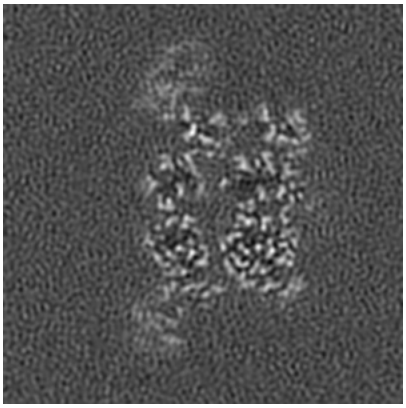
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

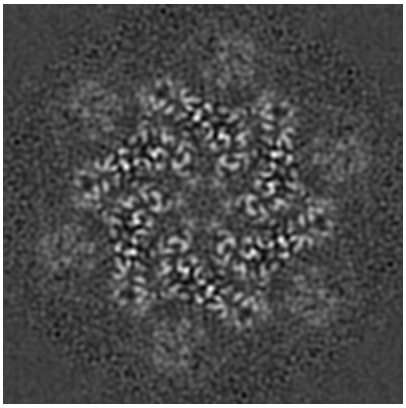
6.3.1 Primary map



X Index: 96



Y Index: 172

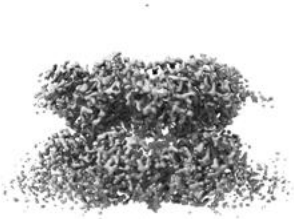


Z Index: 130

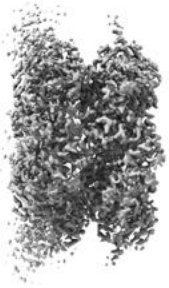
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.0183. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

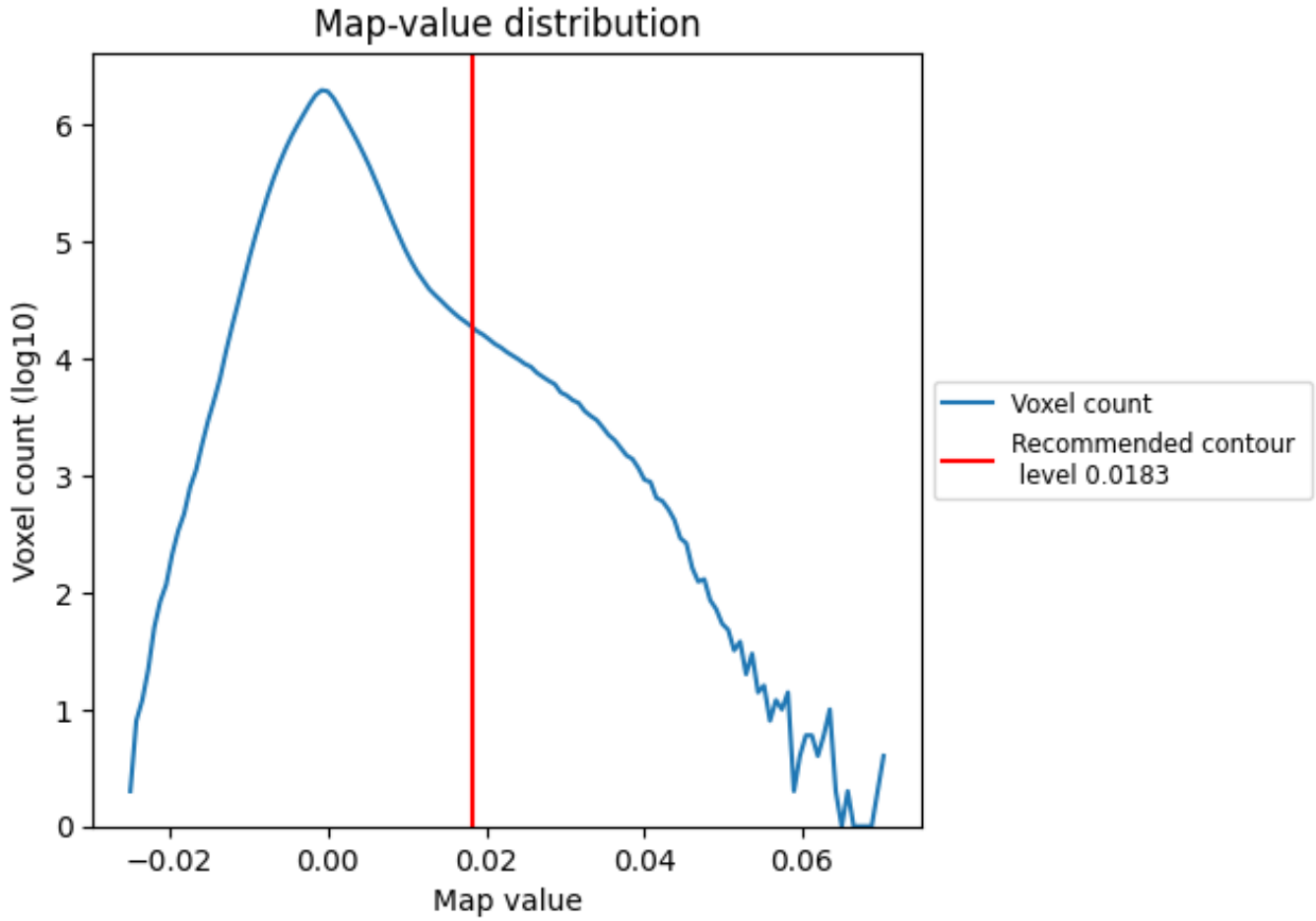
6.5 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

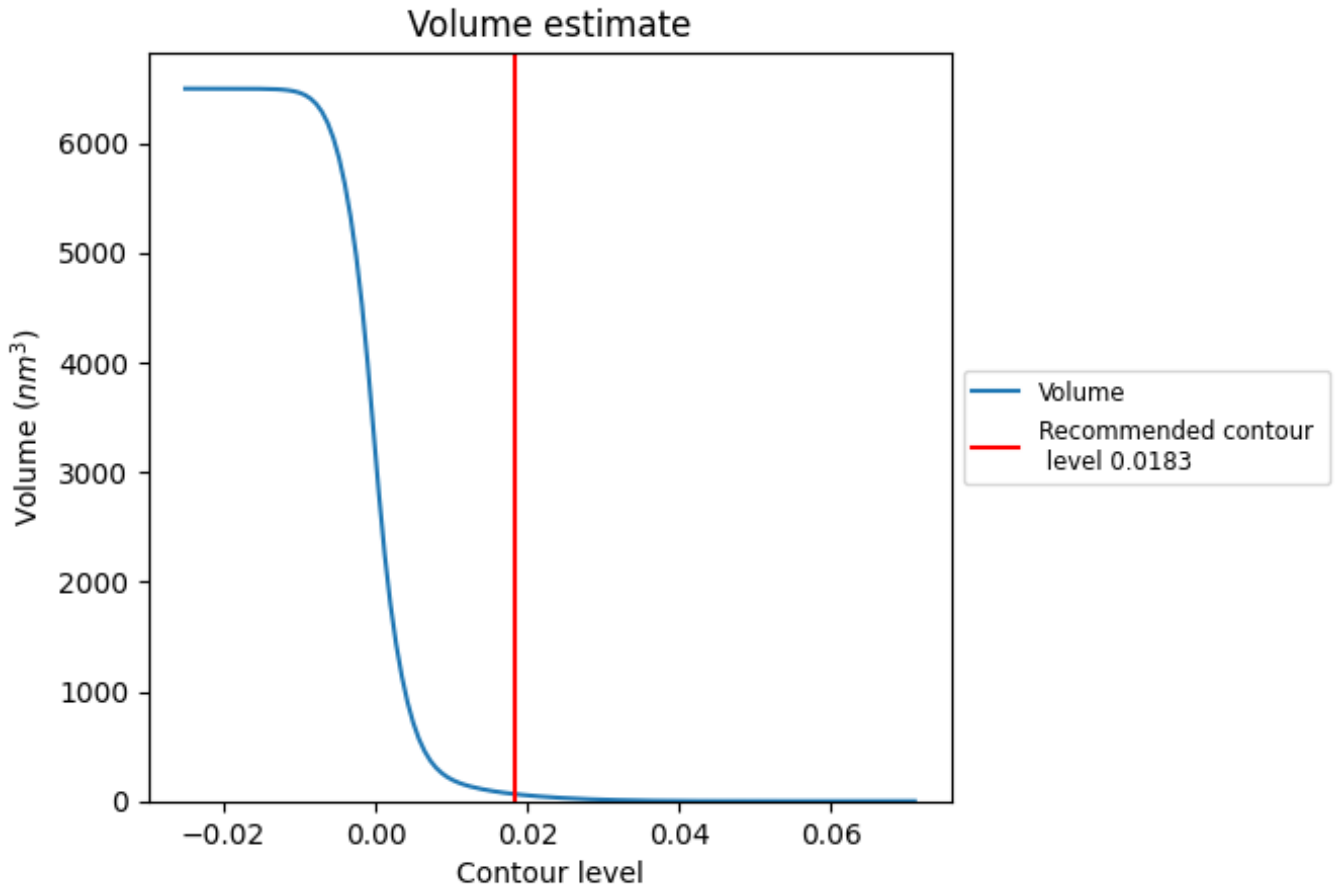
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

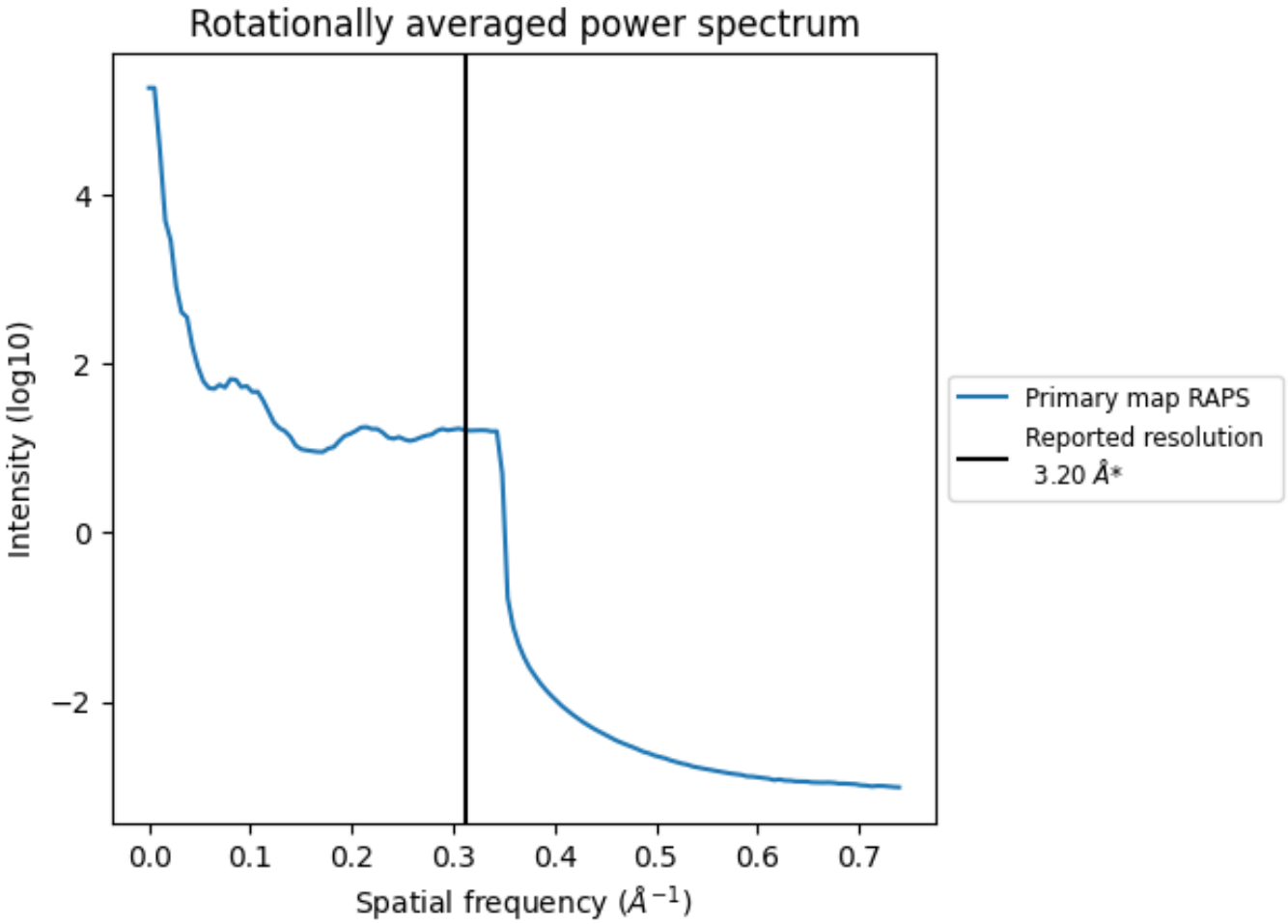
7.2 Volume estimate (i)



The volume at the recommended contour level is 65 nm^3; this corresponds to an approximate mass of 59 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.312 Å^{-1}

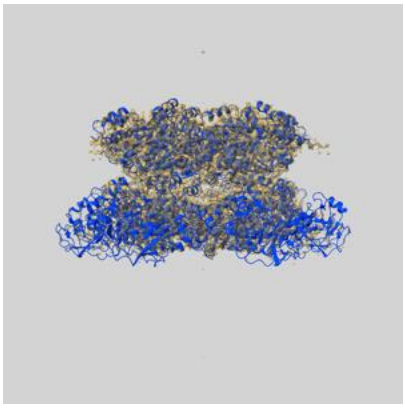
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

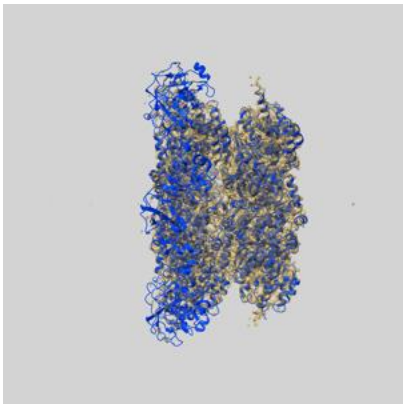
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3298 and PDB model 5FTM. Per-residue inclusion information can be found in section 3 on page 6.

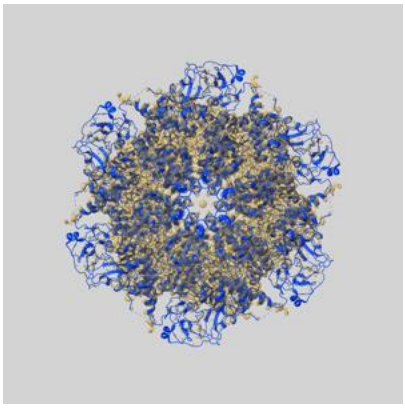
9.1 Map-model overlay



X



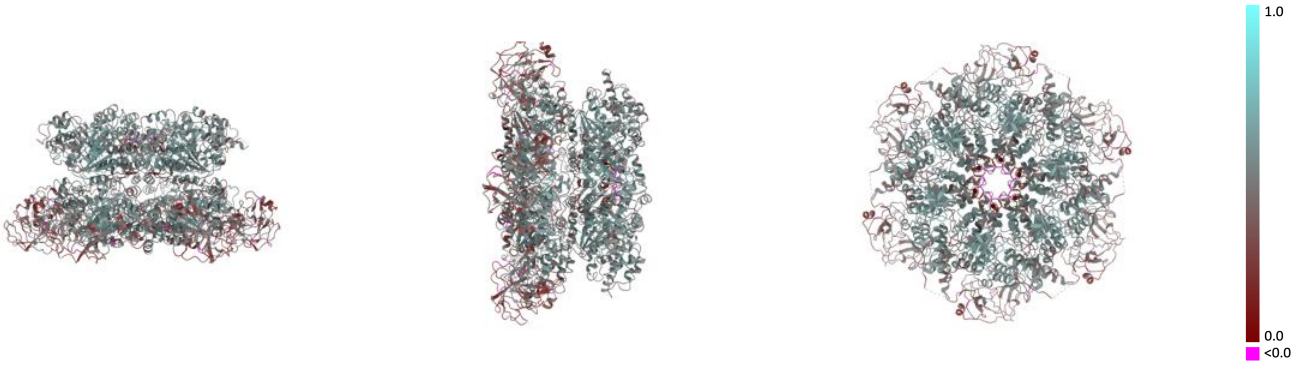
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0183 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

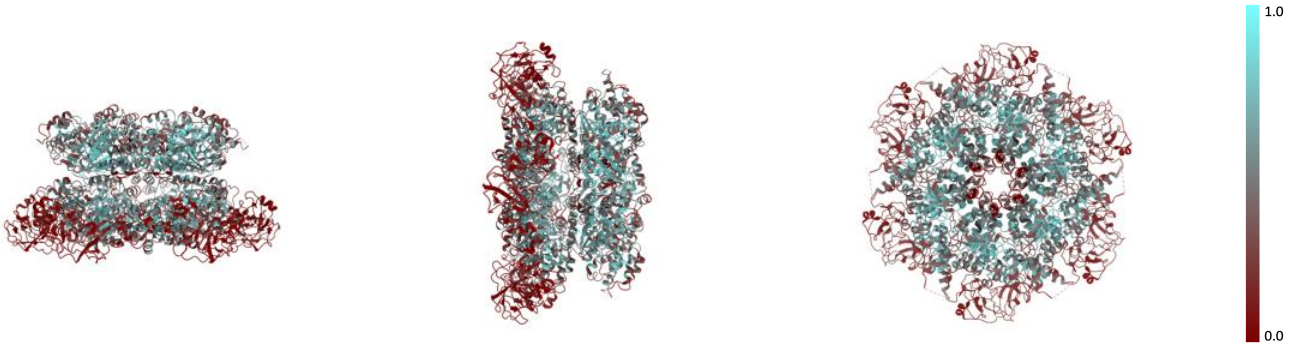
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

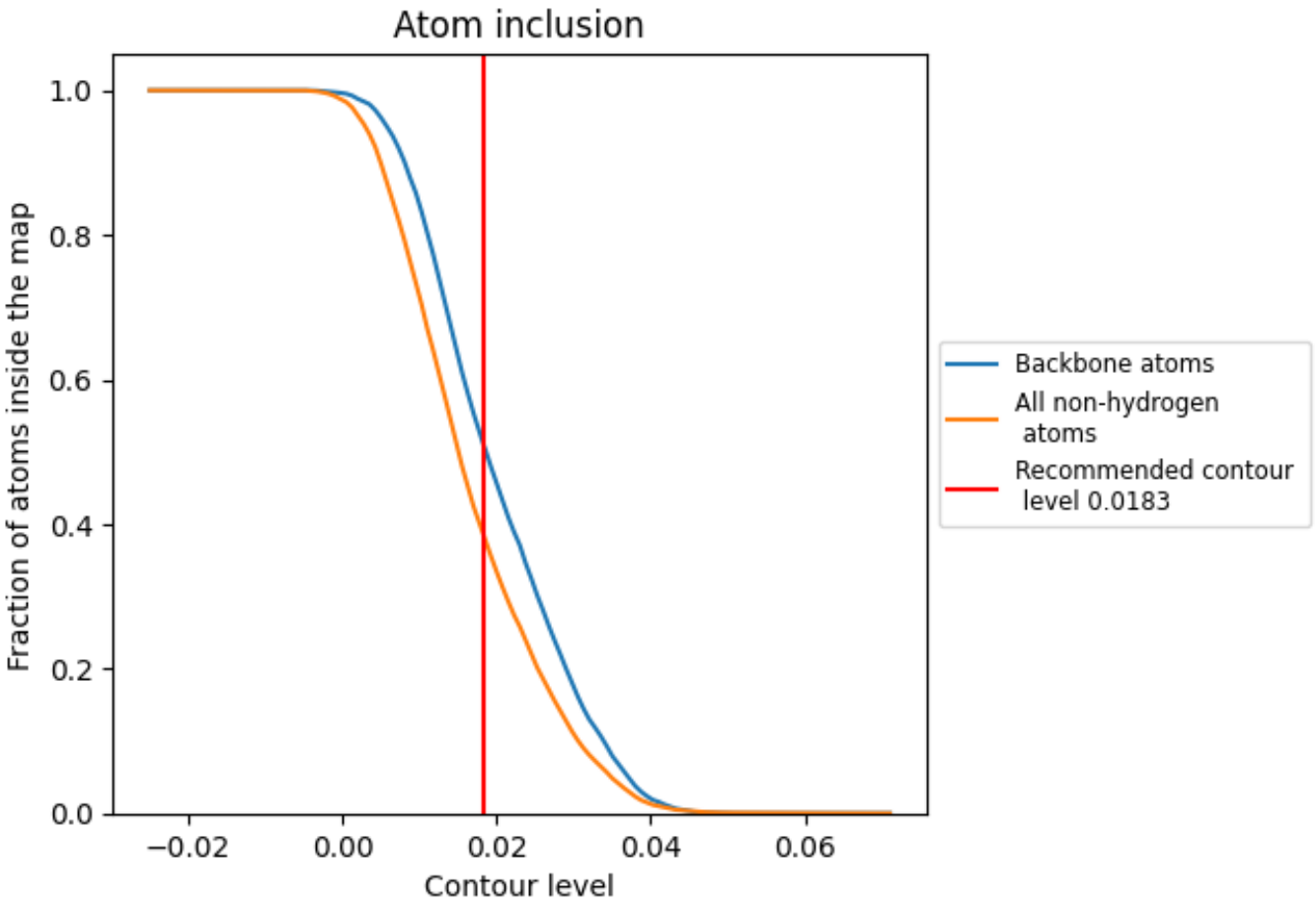
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0183).

9.4 Atom inclusion (i)



At the recommended contour level, 51% of all backbone atoms, 38% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.0183) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.3849	0.4570
A	0.3838	0.4570
B	0.3855	0.4570
C	0.3857	0.4560
D	0.3838	0.4560
E	0.3852	0.4570
F	0.3857	0.4580