wwPDB EM Validation Summary Report (i)

Jun 4, 2025 – 12:25 PM EDT

PDB ID	:	7RLI / pdb_00007rli
EMDB ID	:	EMD-24531
Title	:	Cryo-EM structure of human p97 bound to CB-5083 and ADP.
Authors	:	Caffrey, B.; Zhu, X.; Berezuk, A.; Tuttle, K.; Chittori, S.; Subramaniam, S.
Deposited on	:	2021-07-23
Resolution	:	3.10 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:

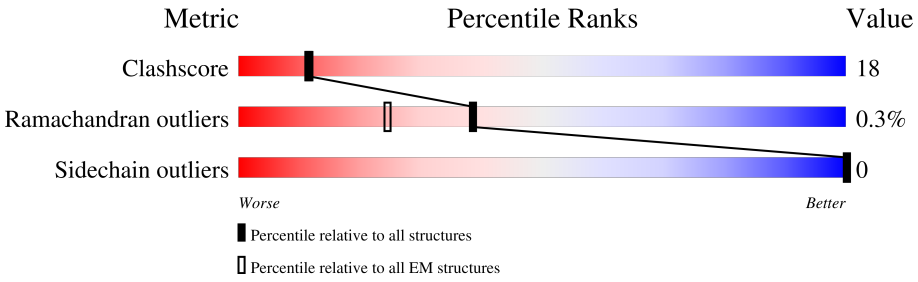
EMDB validation analysis	:	0.0.1.dev118
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0rc1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

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 3.10 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	821	26% 60% 29% 10%
1	B	821	26% 60% 29% 10%
1	C	821	25% 60% 29% 10%
1	D	821	26% 60% 29% 10%
1	E	821	26% 60% 30% 10%
1	F	821	26% 60% 29% 10%
1	G	821	26% 60% 29% 10%
1	H	821	26% 60% 29% 10%

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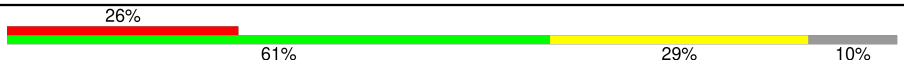
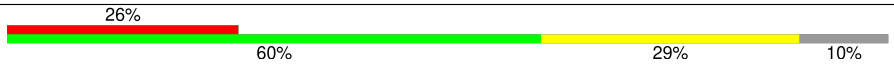
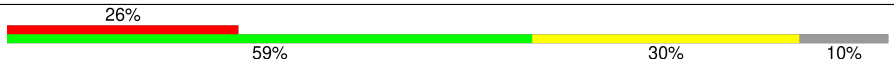
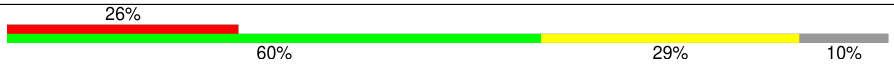
Mol	Chain	Length	Quality of chain
1	I	821	
1	J	821	
1	K	821	
1	L	821	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 69768 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	735	Total 5756	C 3623	N 1015	O 1088	S 30	0	0
1	B	735	Total 5756	C 3623	N 1015	O 1088	S 30	0	0
1	C	735	Total 5756	C 3623	N 1015	O 1088	S 30	0	0
1	D	735	Total 5756	C 3623	N 1015	O 1088	S 30	0	0
1	E	735	Total 5756	C 3623	N 1015	O 1088	S 30	0	0
1	F	735	Total 5756	C 3623	N 1015	O 1088	S 30	0	0
1	G	735	Total 5756	C 3623	N 1015	O 1088	S 30	0	0
1	H	735	Total 5756	C 3623	N 1015	O 1088	S 30	0	0
1	I	735	Total 5756	C 3623	N 1015	O 1088	S 30	0	0
1	J	735	Total 5756	C 3623	N 1015	O 1088	S 30	0	0
1	K	735	Total 5756	C 3623	N 1015	O 1088	S 30	0	0
1	L	735	Total 5756	C 3623	N 1015	O 1088	S 30	0	0

There are 192 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	HIS	-	expression tag	UNP P55072
A	-13	HIS	-	expression tag	UNP P55072
A	-12	HIS	-	expression tag	UNP P55072
A	-11	HIS	-	expression tag	UNP P55072
A	-10	HIS	-	expression tag	UNP P55072
A	-9	HIS	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	GLY	-	expression tag	UNP P55072
A	-7	THR	-	expression tag	UNP P55072
A	-6	SER	-	expression tag	UNP P55072
A	-5	GLU	-	expression tag	UNP P55072
A	-4	ASN	-	expression tag	UNP P55072
A	-3	LEU	-	expression tag	UNP P55072
A	-2	TYR	-	expression tag	UNP P55072
A	-1	PHE	-	expression tag	UNP P55072
A	0	GLN	-	expression tag	UNP P55072
A	1	GLY	-	expression tag	UNP P55072
B	-14	HIS	-	expression tag	UNP P55072
B	-13	HIS	-	expression tag	UNP P55072
B	-12	HIS	-	expression tag	UNP P55072
B	-11	HIS	-	expression tag	UNP P55072
B	-10	HIS	-	expression tag	UNP P55072
B	-9	HIS	-	expression tag	UNP P55072
B	-8	GLY	-	expression tag	UNP P55072
B	-7	THR	-	expression tag	UNP P55072
B	-6	SER	-	expression tag	UNP P55072
B	-5	GLU	-	expression tag	UNP P55072
B	-4	ASN	-	expression tag	UNP P55072
B	-3	LEU	-	expression tag	UNP P55072
B	-2	TYR	-	expression tag	UNP P55072
B	-1	PHE	-	expression tag	UNP P55072
B	0	GLN	-	expression tag	UNP P55072
B	1	GLY	-	expression tag	UNP P55072
C	-14	HIS	-	expression tag	UNP P55072
C	-13	HIS	-	expression tag	UNP P55072
C	-12	HIS	-	expression tag	UNP P55072
C	-11	HIS	-	expression tag	UNP P55072
C	-10	HIS	-	expression tag	UNP P55072
C	-9	HIS	-	expression tag	UNP P55072
C	-8	GLY	-	expression tag	UNP P55072
C	-7	THR	-	expression tag	UNP P55072
C	-6	SER	-	expression tag	UNP P55072
C	-5	GLU	-	expression tag	UNP P55072
C	-4	ASN	-	expression tag	UNP P55072
C	-3	LEU	-	expression tag	UNP P55072
C	-2	TYR	-	expression tag	UNP P55072
C	-1	PHE	-	expression tag	UNP P55072
C	0	GLN	-	expression tag	UNP P55072
C	1	GLY	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	HIS	-	expression tag	UNP P55072
D	-13	HIS	-	expression tag	UNP P55072
D	-12	HIS	-	expression tag	UNP P55072
D	-11	HIS	-	expression tag	UNP P55072
D	-10	HIS	-	expression tag	UNP P55072
D	-9	HIS	-	expression tag	UNP P55072
D	-8	GLY	-	expression tag	UNP P55072
D	-7	THR	-	expression tag	UNP P55072
D	-6	SER	-	expression tag	UNP P55072
D	-5	GLU	-	expression tag	UNP P55072
D	-4	ASN	-	expression tag	UNP P55072
D	-3	LEU	-	expression tag	UNP P55072
D	-2	TYR	-	expression tag	UNP P55072
D	-1	PHE	-	expression tag	UNP P55072
D	0	GLN	-	expression tag	UNP P55072
D	1	GLY	-	expression tag	UNP P55072
E	-14	HIS	-	expression tag	UNP P55072
E	-13	HIS	-	expression tag	UNP P55072
E	-12	HIS	-	expression tag	UNP P55072
E	-11	HIS	-	expression tag	UNP P55072
E	-10	HIS	-	expression tag	UNP P55072
E	-9	HIS	-	expression tag	UNP P55072
E	-8	GLY	-	expression tag	UNP P55072
E	-7	THR	-	expression tag	UNP P55072
E	-6	SER	-	expression tag	UNP P55072
E	-5	GLU	-	expression tag	UNP P55072
E	-4	ASN	-	expression tag	UNP P55072
E	-3	LEU	-	expression tag	UNP P55072
E	-2	TYR	-	expression tag	UNP P55072
E	-1	PHE	-	expression tag	UNP P55072
E	0	GLN	-	expression tag	UNP P55072
E	1	GLY	-	expression tag	UNP P55072
F	-14	HIS	-	expression tag	UNP P55072
F	-13	HIS	-	expression tag	UNP P55072
F	-12	HIS	-	expression tag	UNP P55072
F	-11	HIS	-	expression tag	UNP P55072
F	-10	HIS	-	expression tag	UNP P55072
F	-9	HIS	-	expression tag	UNP P55072
F	-8	GLY	-	expression tag	UNP P55072
F	-7	THR	-	expression tag	UNP P55072
F	-6	SER	-	expression tag	UNP P55072
F	-5	GLU	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-4	ASN	-	expression tag	UNP P55072
F	-3	LEU	-	expression tag	UNP P55072
F	-2	TYR	-	expression tag	UNP P55072
F	-1	PHE	-	expression tag	UNP P55072
F	0	GLN	-	expression tag	UNP P55072
F	1	GLY	-	expression tag	UNP P55072
G	-14	HIS	-	expression tag	UNP P55072
G	-13	HIS	-	expression tag	UNP P55072
G	-12	HIS	-	expression tag	UNP P55072
G	-11	HIS	-	expression tag	UNP P55072
G	-10	HIS	-	expression tag	UNP P55072
G	-9	HIS	-	expression tag	UNP P55072
G	-8	GLY	-	expression tag	UNP P55072
G	-7	THR	-	expression tag	UNP P55072
G	-6	SER	-	expression tag	UNP P55072
G	-5	GLU	-	expression tag	UNP P55072
G	-4	ASN	-	expression tag	UNP P55072
G	-3	LEU	-	expression tag	UNP P55072
G	-2	TYR	-	expression tag	UNP P55072
G	-1	PHE	-	expression tag	UNP P55072
G	0	GLN	-	expression tag	UNP P55072
G	1	GLY	-	expression tag	UNP P55072
H	-14	HIS	-	expression tag	UNP P55072
H	-13	HIS	-	expression tag	UNP P55072
H	-12	HIS	-	expression tag	UNP P55072
H	-11	HIS	-	expression tag	UNP P55072
H	-10	HIS	-	expression tag	UNP P55072
H	-9	HIS	-	expression tag	UNP P55072
H	-8	GLY	-	expression tag	UNP P55072
H	-7	THR	-	expression tag	UNP P55072
H	-6	SER	-	expression tag	UNP P55072
H	-5	GLU	-	expression tag	UNP P55072
H	-4	ASN	-	expression tag	UNP P55072
H	-3	LEU	-	expression tag	UNP P55072
H	-2	TYR	-	expression tag	UNP P55072
H	-1	PHE	-	expression tag	UNP P55072
H	0	GLN	-	expression tag	UNP P55072
H	1	GLY	-	expression tag	UNP P55072
I	-14	HIS	-	expression tag	UNP P55072
I	-13	HIS	-	expression tag	UNP P55072
I	-12	HIS	-	expression tag	UNP P55072
I	-11	HIS	-	expression tag	UNP P55072

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-10	HIS	-	expression tag	UNP P55072
I	-9	HIS	-	expression tag	UNP P55072
I	-8	GLY	-	expression tag	UNP P55072
I	-7	THR	-	expression tag	UNP P55072
I	-6	SER	-	expression tag	UNP P55072
I	-5	GLU	-	expression tag	UNP P55072
I	-4	ASN	-	expression tag	UNP P55072
I	-3	LEU	-	expression tag	UNP P55072
I	-2	TYR	-	expression tag	UNP P55072
I	-1	PHE	-	expression tag	UNP P55072
I	0	GLN	-	expression tag	UNP P55072
I	1	GLY	-	expression tag	UNP P55072
J	-14	HIS	-	expression tag	UNP P55072
J	-13	HIS	-	expression tag	UNP P55072
J	-12	HIS	-	expression tag	UNP P55072
J	-11	HIS	-	expression tag	UNP P55072
J	-10	HIS	-	expression tag	UNP P55072
J	-9	HIS	-	expression tag	UNP P55072
J	-8	GLY	-	expression tag	UNP P55072
J	-7	THR	-	expression tag	UNP P55072
J	-6	SER	-	expression tag	UNP P55072
J	-5	GLU	-	expression tag	UNP P55072
J	-4	ASN	-	expression tag	UNP P55072
J	-3	LEU	-	expression tag	UNP P55072
J	-2	TYR	-	expression tag	UNP P55072
J	-1	PHE	-	expression tag	UNP P55072
J	0	GLN	-	expression tag	UNP P55072
J	1	GLY	-	expression tag	UNP P55072
K	-14	HIS	-	expression tag	UNP P55072
K	-13	HIS	-	expression tag	UNP P55072
K	-12	HIS	-	expression tag	UNP P55072
K	-11	HIS	-	expression tag	UNP P55072
K	-10	HIS	-	expression tag	UNP P55072
K	-9	HIS	-	expression tag	UNP P55072
K	-8	GLY	-	expression tag	UNP P55072
K	-7	THR	-	expression tag	UNP P55072
K	-6	SER	-	expression tag	UNP P55072
K	-5	GLU	-	expression tag	UNP P55072
K	-4	ASN	-	expression tag	UNP P55072
K	-3	LEU	-	expression tag	UNP P55072
K	-2	TYR	-	expression tag	UNP P55072
K	-1	PHE	-	expression tag	UNP P55072

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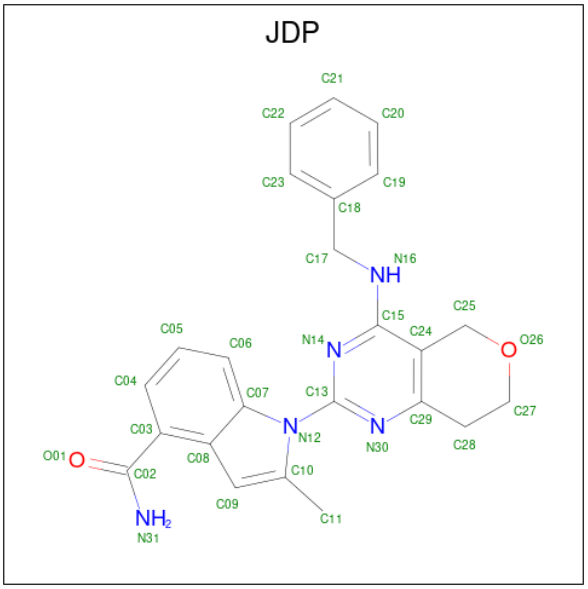
Chain	Residue	Modelled	Actual	Comment	Reference
K	0	GLN	-	expression tag	UNP P55072
K	1	GLY	-	expression tag	UNP P55072
L	-14	HIS	-	expression tag	UNP P55072
L	-13	HIS	-	expression tag	UNP P55072
L	-12	HIS	-	expression tag	UNP P55072
L	-11	HIS	-	expression tag	UNP P55072
L	-10	HIS	-	expression tag	UNP P55072
L	-9	HIS	-	expression tag	UNP P55072
L	-8	GLY	-	expression tag	UNP P55072
L	-7	THR	-	expression tag	UNP P55072
L	-6	SER	-	expression tag	UNP P55072
L	-5	GLU	-	expression tag	UNP P55072
L	-4	ASN	-	expression tag	UNP P55072
L	-3	LEU	-	expression tag	UNP P55072
L	-2	TYR	-	expression tag	UNP P55072
L	-1	PHE	-	expression tag	UNP P55072
L	0	GLN	-	expression tag	UNP P55072
L	1	GLY	-	expression tag	UNP P55072

- Molecule 2 is 1-[4-(benzylamino)-7,8-dihydro-5H-pyrano[4,3-d]pyrimidin-2-yl]-2-methyl -1H-indole-4-carboxamide (CCD ID: JDP) (formula: $C_{24}H_{23}N_5O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			31	24	5	2	

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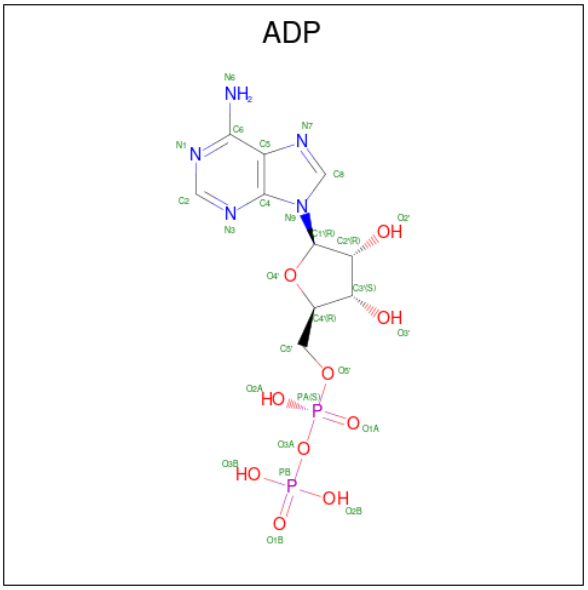
Mol	Chain	Residues	Atoms				AltConf
2	B	1	Total	C	N	O	0
			31	24	5	2	
2	C	1	Total	C	N	O	0
			31	24	5	2	
2	D	1	Total	C	N	O	0
			31	24	5	2	
2	E	1	Total	C	N	O	0
			31	24	5	2	
2	F	1	Total	C	N	O	0
			31	24	5	2	
2	G	1	Total	C	N	O	0
			31	24	5	2	
2	H	1	Total	C	N	O	0
			31	24	5	2	
2	I	1	Total	C	N	O	0
			31	24	5	2	
2	J	1	Total	C	N	O	0
			31	24	5	2	
2	K	1	Total	C	N	O	0
			31	24	5	2	
2	L	1	Total	C	N	O	0
			31	24	5	2	

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



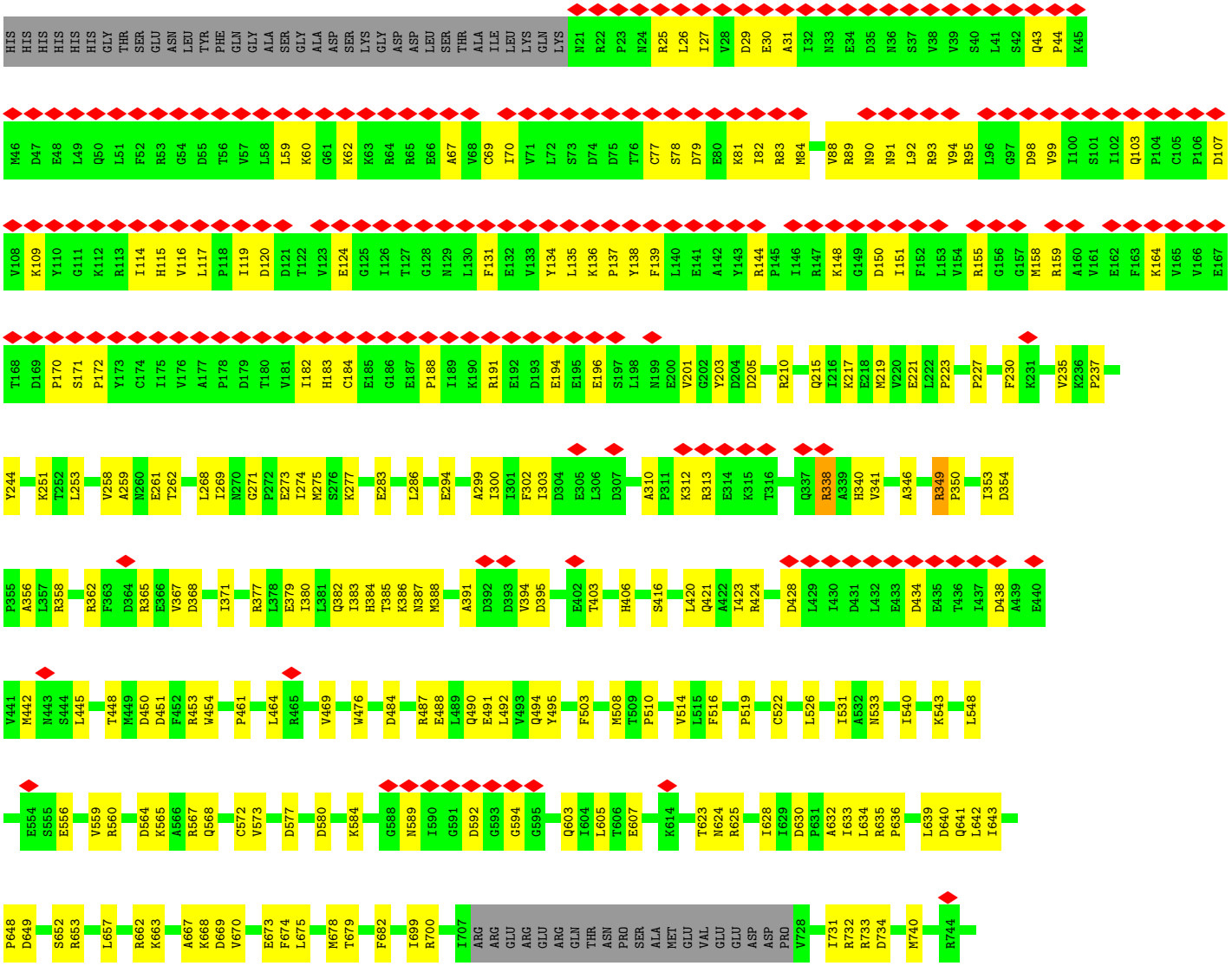
Mol	Chain	Residues	Atoms					AltConf
3	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	C	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	D	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	F	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	I	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	J	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	K	1	Total	C	N	O	P	0
			27	10	5	10	2	
3	L	1	Total	C	N	O	P	0
			27	10	5	10	2	

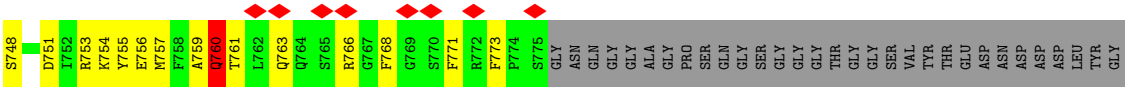
3 Residue-property plots (i)

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

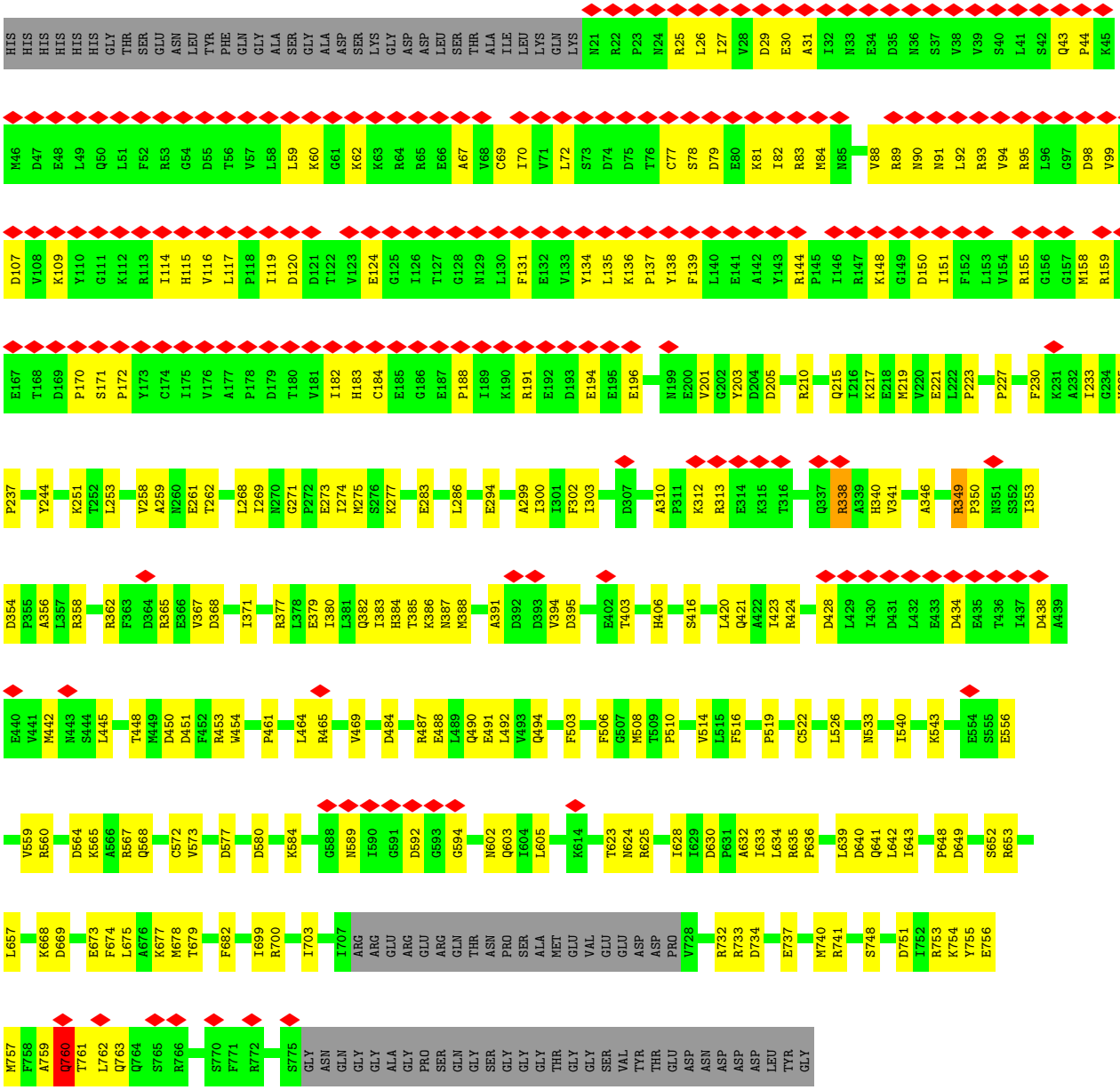
Chain A:





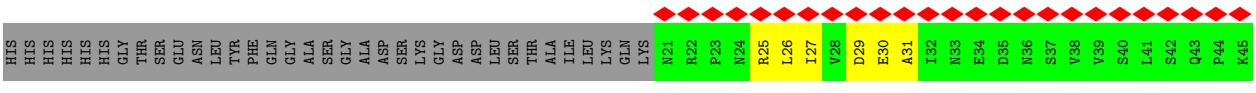
• Molecule 1: Transitional endoplasmic reticulum ATPase

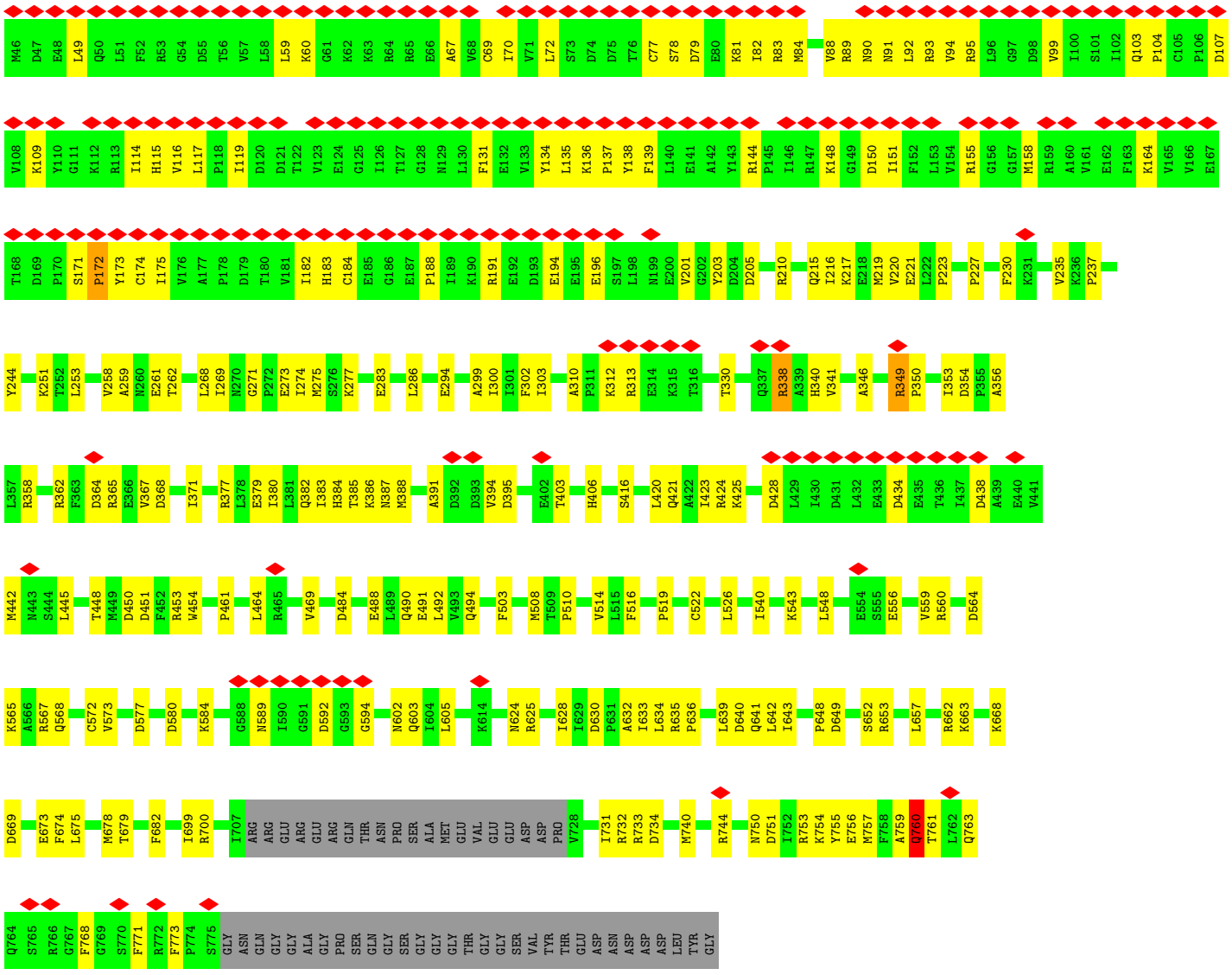
Chain B:



• Molecule 1: Transitional endoplasmic reticulum ATPase

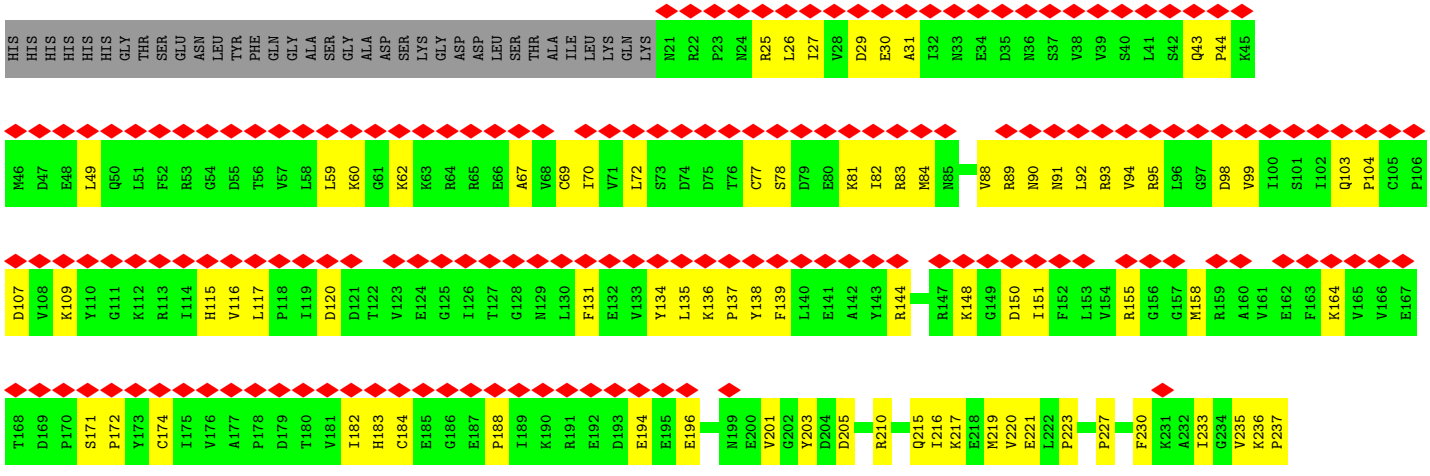
Chain C:

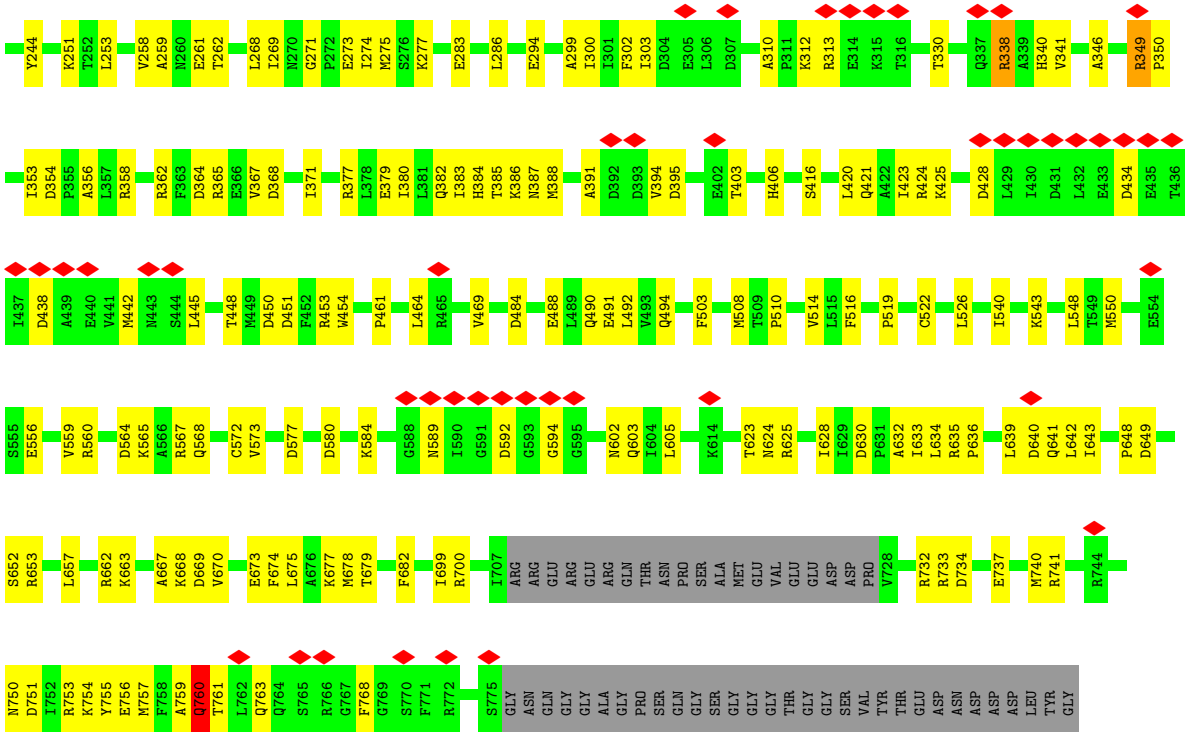




• Molecule 1: Transitional endoplasmic reticulum ATPase

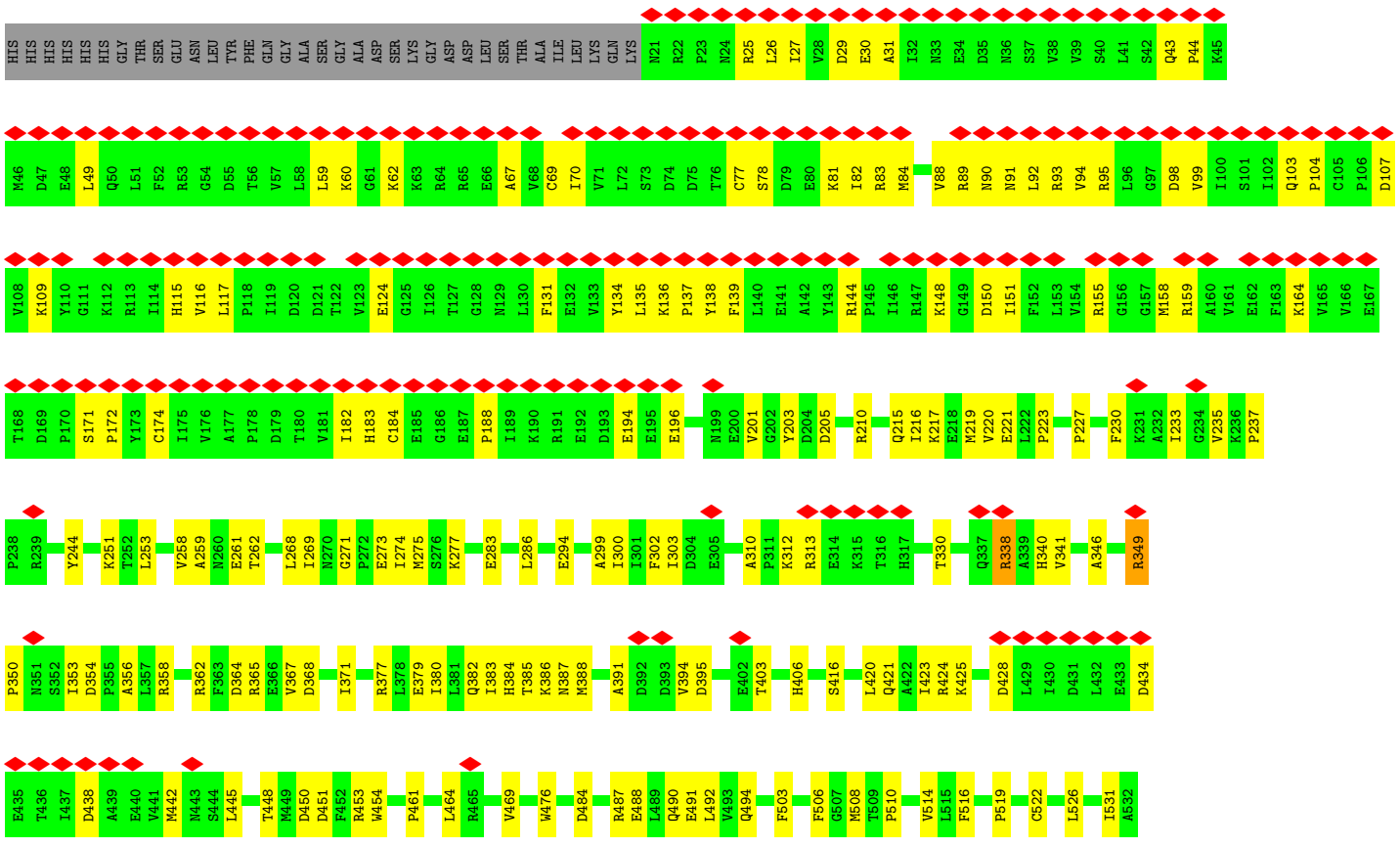
Chain D:

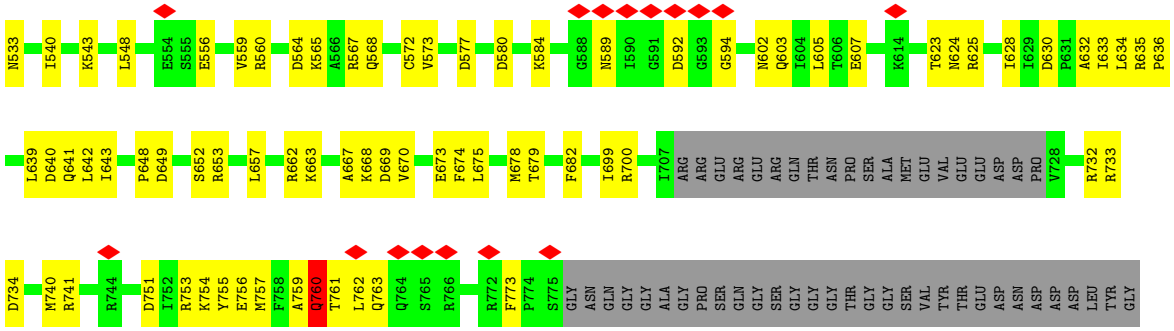




• Molecule 1: Transitional endoplasmic reticulum ATPase

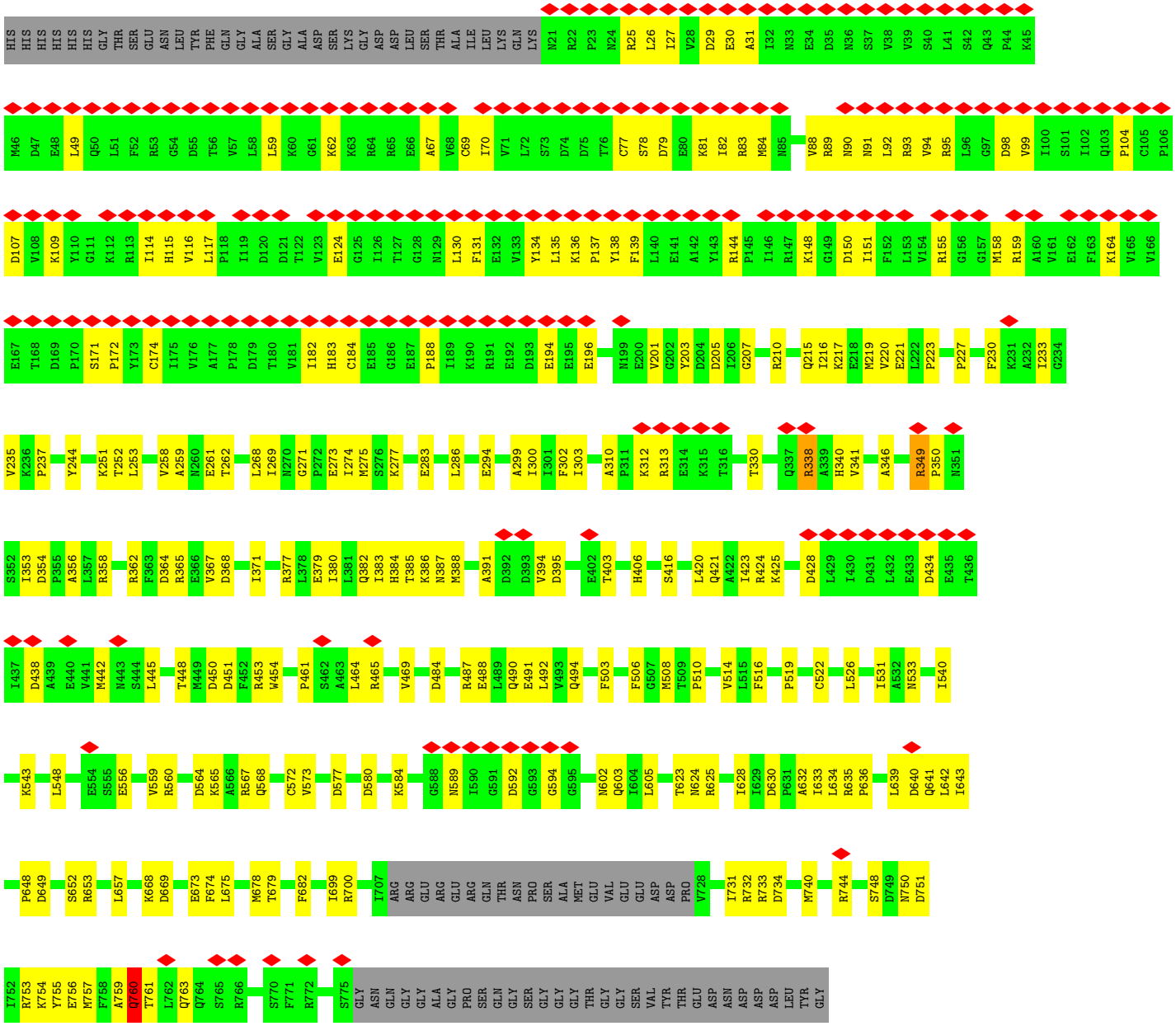
Chain E:





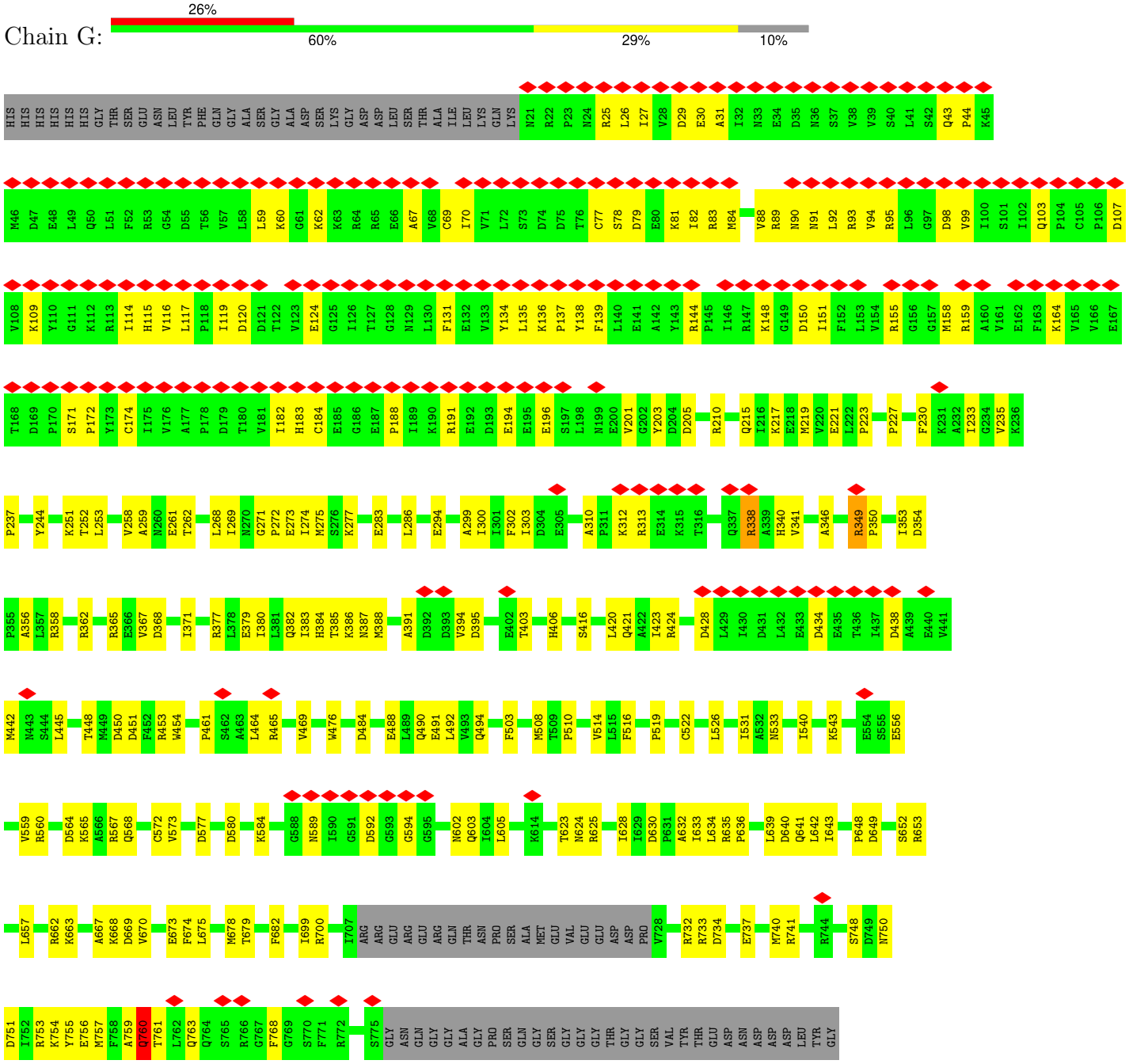
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain F:



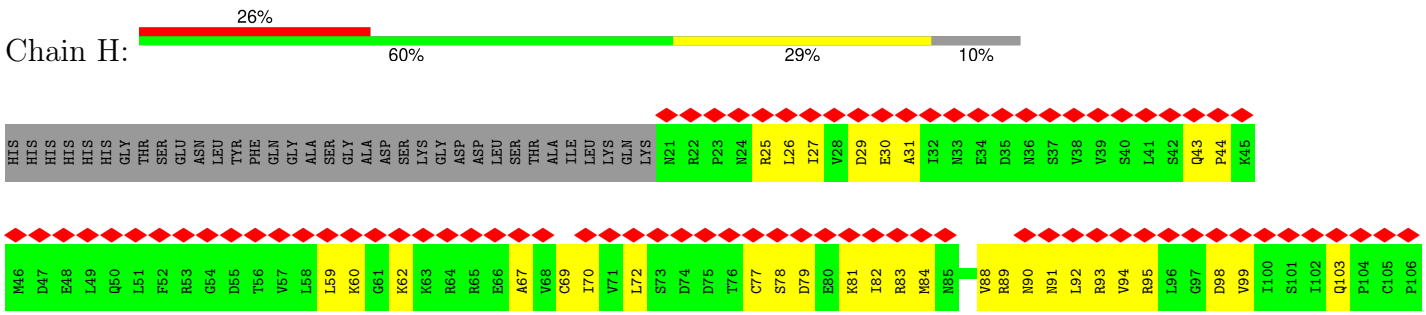
• Molecule 1: Transitional endoplasmic reticulum ATPase

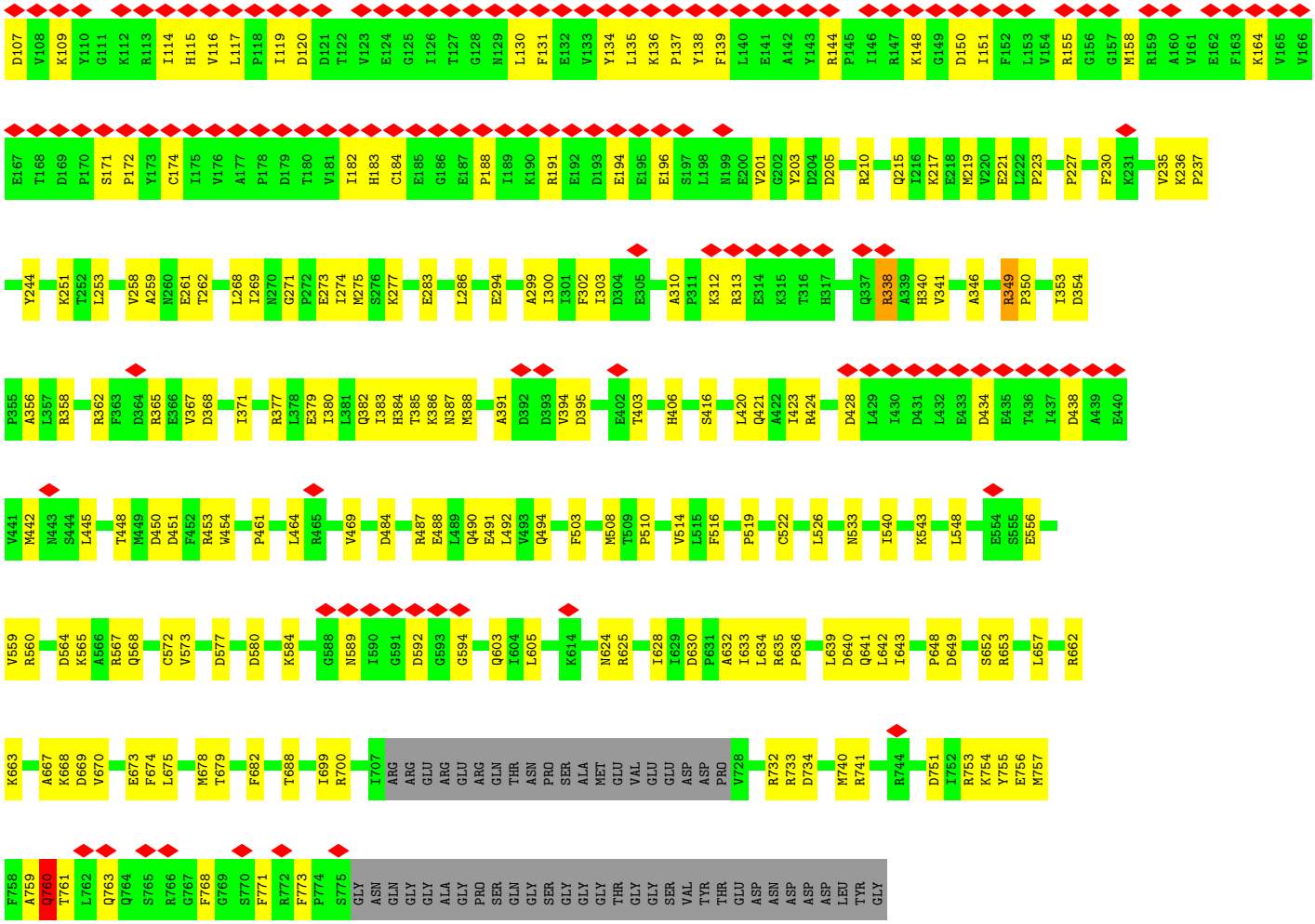
Chain G:



• Molecule 1: Transitional endoplasmic reticulum ATPase

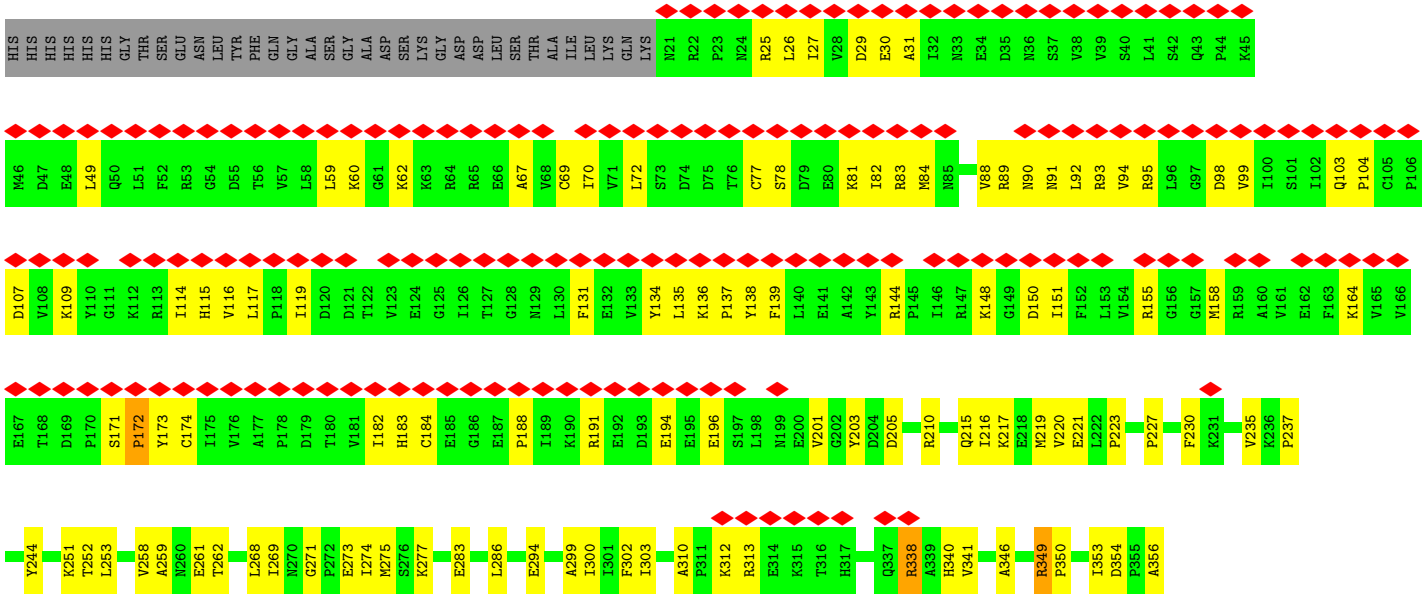
Chain H:

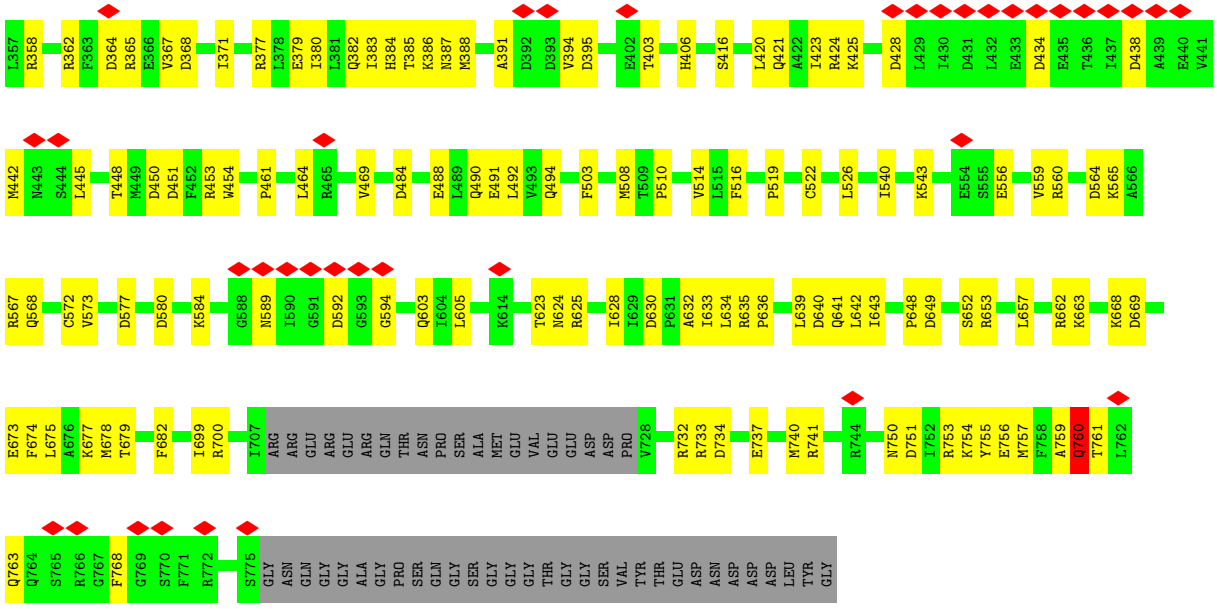




• Molecule 1: Transitional endoplasmic reticulum ATPase

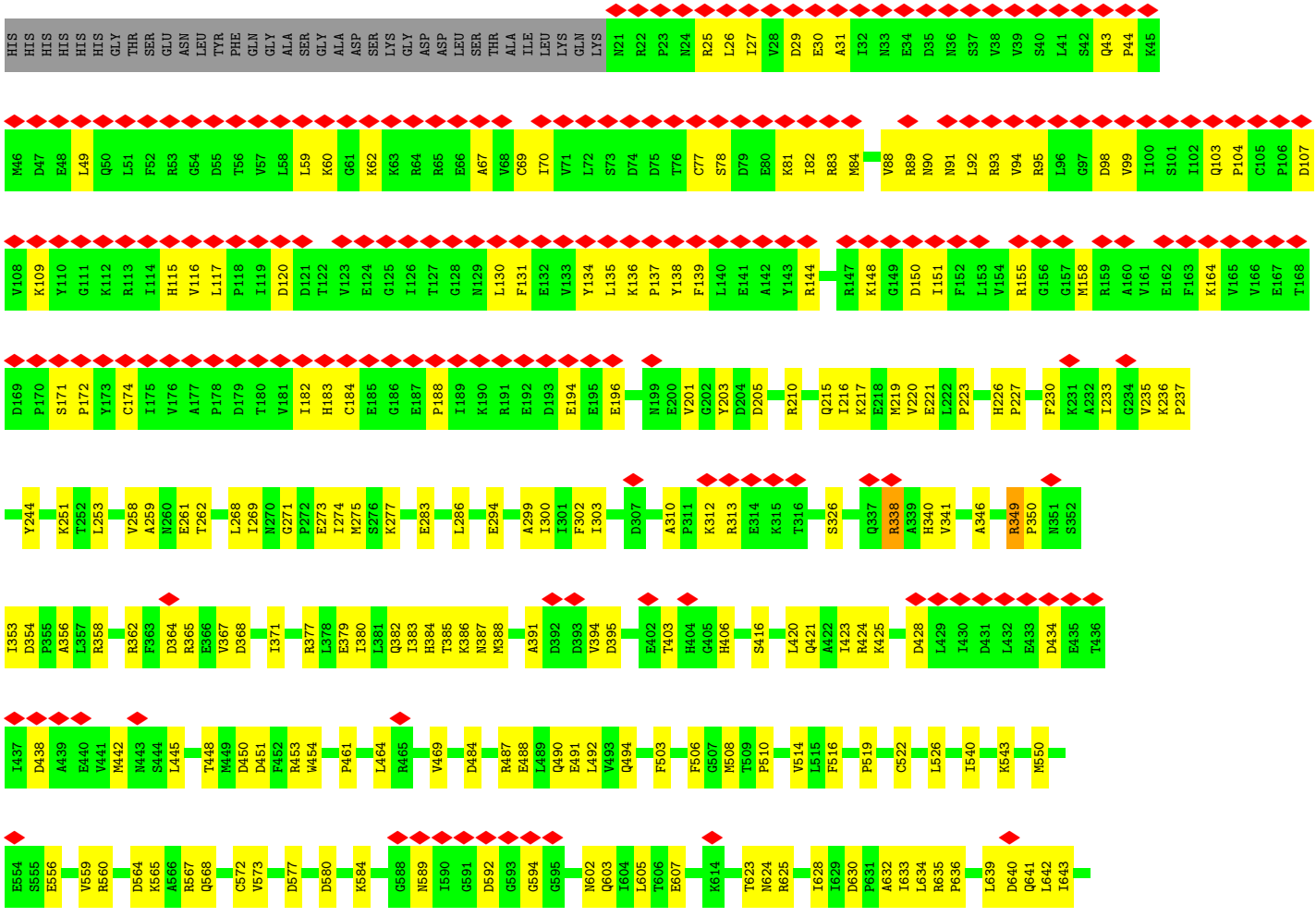
Chain I:

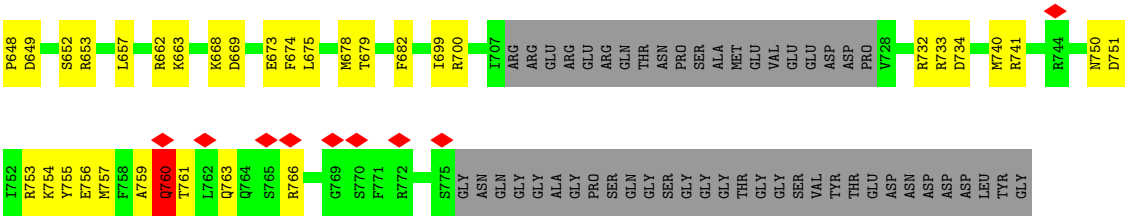




• Molecule 1: Transitional endoplasmic reticulum ATPase

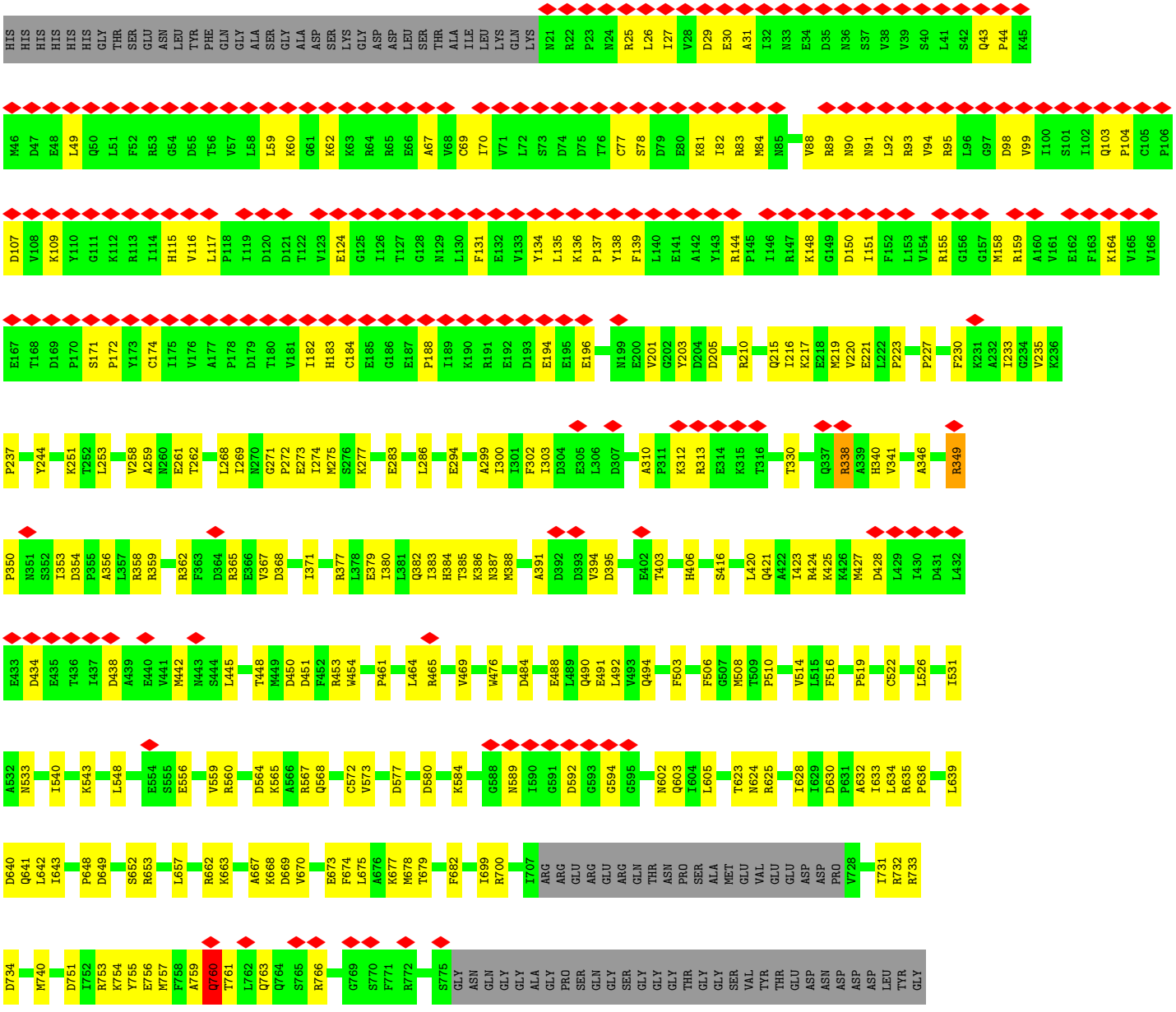
Chain J:





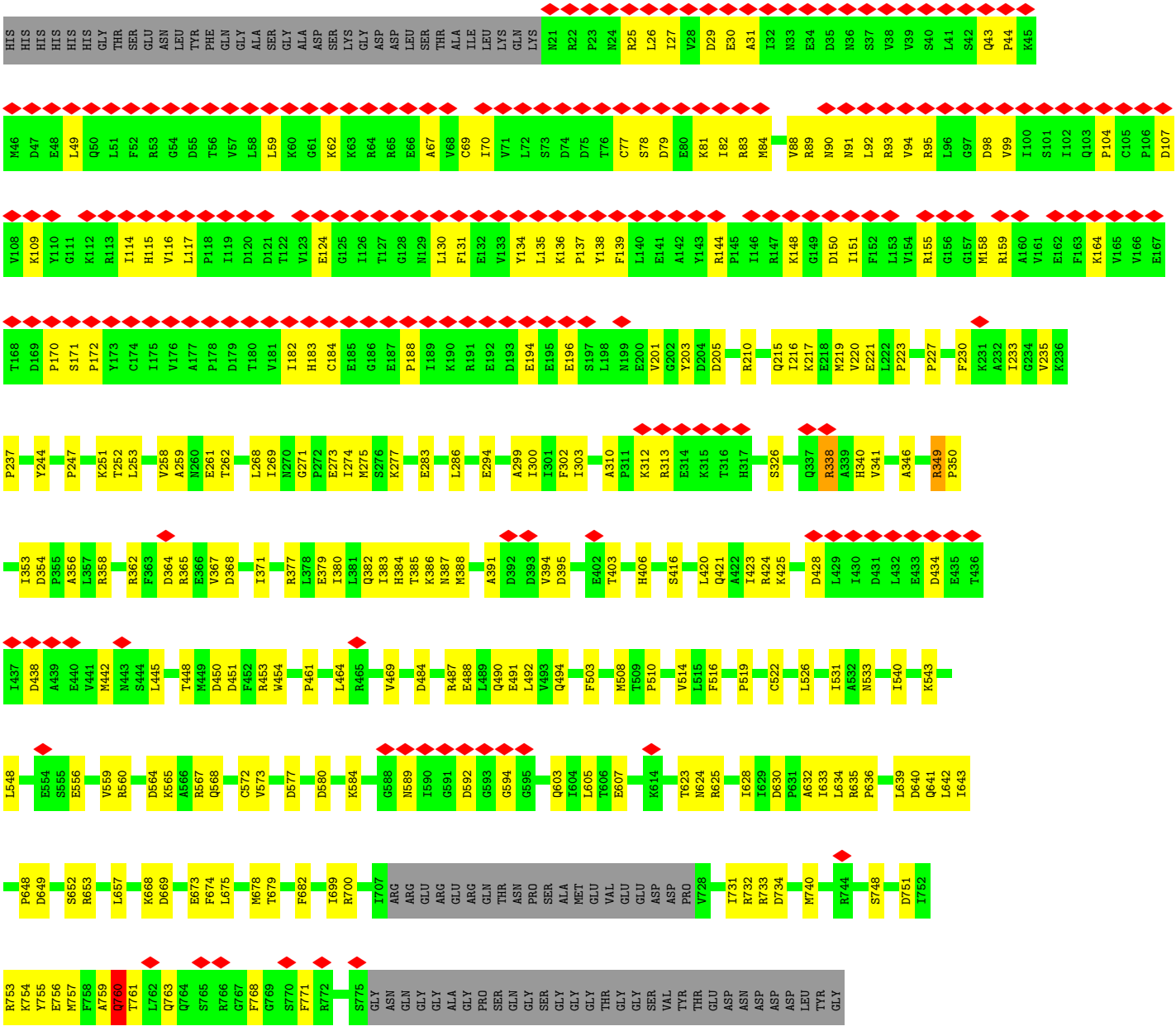
• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain K:



• Molecule 1: Transitional endoplasmic reticulum ATPase

Chain L:


HIS HIS HIS HIS HIS HIS GLY THR SER GLU ASN LEU TYR PHE GLN GLY 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 M36 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 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 V201 G202 Y203 D204 D205 R210 Q215 I216 K217 E218 M219 V220 E221 L222 P223 P227 F230 K231 A232 I233 G234 V235 K236
P237 Y244 P247 K251 T252 L253 V258 A259 N260 E261 T262 L268 T269 N270 G271 P272 E273 I274 M275 S276 K277 E283 L286 E294 A299 I300 I301 F302 I303 A310 P311 K312 R313 E314 K315 T316 H317 S326 Q337 R338 A339 H340 V341 A346 R349 P350
I353 D354 P355 A356 L357 R358 R362 F363 D364 R365 E366 V367 D368 I371 R377 L378 E379 I380 L381 Q382 I383 H384 T385 K386 N387 M388 A391 D392 D393 V394 D395 E402 T403 H406 S416 L420 Q421 A422 I423 R424 K425 D428 L429 I430 D431 L432 E433 D434 E435 T436
I437 D438 A439 E440 V441 M442 N443 S444 L445 T448 M449 D450 D451 F452 R453 W454 P461 L464 R465 V469 D484 R487 E488 L489 Q490 E491 L492 V493 Q494 F503 M508 T509 P510 V514 L515 F516 P519 C522 L526 I531 A532 N533 I540 K543
L548 E554 S555 E556 V559 R560 D564 K565 A566 R567 Q568 C572 V573 D577 D580 K584 G588 N589 I590 G591 D592 G593 G594 G595 Q603 I604 L605 T606 E607 K614 T623 N624 R625 I628 I629 D630 P631 A632 I633 L634 R635 P636 L639 D640 Q641 L642 I643
P648 D649 S652 R653 L657 K668 D669 E673 F674 L675 M678 T679 F682 I699 R700 I707 ARG ARG GLU ARG GLU ARG GLN THR ASN PRO SER ALA MET GLU VAL GLU GLU ASP ASP PRO V728 I731 R732 R733 D734 M740 R744 S748 D751 I752
R753 K754 Y755 E756 M757 F758 A759 Q760 T761 L762 Q763 Q764 S765 R766 G767 F768 G769 S770 F771 R772 S775 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, Not provided	
Number of particles used	85876	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.283	Depositor
Minimum map value	-0.308	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.043	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	400.0, 400.0, 400.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.0, 1.0, 1.0	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.17	0/5852	0.45	2/7901 (0.0%)
1	B	0.17	0/5852	0.45	2/7901 (0.0%)
1	C	0.17	0/5852	0.45	2/7901 (0.0%)
1	D	0.17	0/5852	0.45	2/7901 (0.0%)
1	E	0.17	0/5852	0.45	2/7901 (0.0%)
1	F	0.17	0/5852	0.45	2/7901 (0.0%)
1	G	0.17	0/5852	0.45	2/7901 (0.0%)
1	H	0.17	0/5852	0.45	2/7901 (0.0%)
1	I	0.17	0/5852	0.45	2/7901 (0.0%)
1	J	0.17	0/5852	0.45	2/7901 (0.0%)
1	K	0.17	0/5852	0.45	2/7901 (0.0%)
1	L	0.17	0/5852	0.45	2/7901 (0.0%)
All	All	0.17	0/70224	0.45	24/94812 (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
1	G	0	2
1	H	0	2
1	I	0	2
1	J	0	2
1	K	0	2

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	L	0	2
All	All	0	24

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	I	349	ARG	CG-CD-NE	7.24	127.92	112.00
1	J	349	ARG	CG-CD-NE	7.23	127.90	112.00
1	K	349	ARG	CG-CD-NE	7.23	127.90	112.00
1	C	349	ARG	CG-CD-NE	7.23	127.90	112.00
1	E	349	ARG	CG-CD-NE	7.22	127.89	112.00

There are no chirality outliers.

5 of 24 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	349	ARG	Sidechain
1	A	760	GLN	Peptide
1	B	349	ARG	Sidechain
1	B	760	GLN	Peptide
1	C	349	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	5756	0	5819	241	0
1	B	5756	0	5819	240	0
1	C	5756	0	5820	213	0
1	D	5756	0	5820	211	0
1	E	5756	0	5820	212	0
1	F	5756	0	5820	219	0
1	G	5756	0	5820	212	0
1	H	5756	0	5820	218	0
1	I	5756	0	5820	211	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	J	5756	0	5819	213	0
1	K	5756	0	5819	220	0
1	L	5756	0	5820	238	0
2	A	31	0	0	1	0
2	B	31	0	0	1	0
2	C	31	0	0	1	0
2	D	31	0	0	1	0
2	E	31	0	0	1	0
2	F	31	0	0	1	0
2	G	31	0	0	1	0
2	H	31	0	0	2	0
2	I	31	0	0	1	0
2	J	31	0	0	1	0
2	K	31	0	0	1	0
2	L	31	0	0	1	0
3	A	27	0	12	2	0
3	B	27	0	12	0	0
3	C	27	0	12	1	0
3	D	27	0	12	1	0
3	E	27	0	12	0	0
3	F	27	0	12	3	0
3	G	27	0	12	3	0
3	H	27	0	12	1	0
3	I	27	0	12	2	0
3	J	27	0	12	0	0
3	K	27	0	12	1	0
3	L	27	0	12	3	0
All	All	69768	0	69980	2450	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 18.

The worst 5 of 2450 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:A:148:LYS:NZ	1:A:171:SER:H	1.03	1.46
1:B:675:LEU:CD1	1:B:740:MET:HE1	1.45	1.46
1:H:675:LEU:CD1	1:H:740:MET:HE1	1.46	1.46
1:L:148:LYS:NZ	1:L:171:SER:H	1.04	1.46
1:F:760:GLN:HE21	1:L:760:GLN:NE2	0.97	1.45

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	731/821 (89%)	691 (94%)	38 (5%)	2 (0%)	37	68
1	B	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
1	C	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
1	D	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
1	E	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
1	F	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
1	G	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
1	H	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
1	I	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
1	J	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
1	K	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
1	L	731/821 (89%)	690 (94%)	39 (5%)	2 (0%)	37	68
All	All	8772/9852 (89%)	8281 (94%)	467 (5%)	24 (0%)	38	68

5 of 24 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	PRO
1	B	172	PRO
1	C	172	PRO
1	D	172	PRO
1	E	172	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	625/691 (90%)	625 (100%)	0	100	100
1	B	625/691 (90%)	625 (100%)	0	100	100
1	C	625/691 (90%)	625 (100%)	0	100	100
1	D	625/691 (90%)	625 (100%)	0	100	100
1	E	625/691 (90%)	625 (100%)	0	100	100
1	F	625/691 (90%)	625 (100%)	0	100	100
1	G	625/691 (90%)	625 (100%)	0	100	100
1	H	625/691 (90%)	625 (100%)	0	100	100
1	I	625/691 (90%)	625 (100%)	0	100	100
1	J	625/691 (90%)	625 (100%)	0	100	100
1	K	625/691 (90%)	625 (100%)	0	100	100
1	L	625/691 (90%)	625 (100%)	0	100	100
All	All	7500/8292 (90%)	7500 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 81 such sidechains are listed below:

Mol	Chain	Res	Type
1	I	764	GLN
1	K	764	GLN
1	J	285	ASN
1	J	764	GLN
1	L	384	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ADP	A	902	-	24,29,29	0.87	0	29,45,45	1.16	2 (6%)
3	ADP	K	902	-	24,29,29	0.88	0	29,45,45	1.17	2 (6%)
2	JDP	I	901	-	33,35,35	2.17	6 (18%)	32,50,50	3.13	7 (21%)
3	ADP	I	902	-	24,29,29	0.89	0	29,45,45	1.16	2 (6%)
2	JDP	B	901	-	33,35,35	2.19	6 (18%)	32,50,50	3.12	7 (21%)
3	ADP	F	902	-	24,29,29	0.88	0	29,45,45	1.17	2 (6%)
3	ADP	B	902	-	24,29,29	0.88	0	29,45,45	1.17	2 (6%)
2	JDP	E	901	-	33,35,35	2.18	6 (18%)	32,50,50	3.12	8 (25%)
2	JDP	A	901	-	33,35,35	2.19	6 (18%)	32,50,50	3.13	7 (21%)
3	ADP	E	902	-	24,29,29	0.87	0	29,45,45	1.17	2 (6%)
2	JDP	J	901	-	33,35,35	2.18	6 (18%)	32,50,50	3.12	7 (21%)
2	JDP	F	901	-	33,35,35	2.18	6 (18%)	32,50,50	3.12	7 (21%)
3	ADP	L	902	-	24,29,29	0.87	0	29,45,45	1.17	2 (6%)
3	ADP	G	902	-	24,29,29	0.89	0	29,45,45	1.17	2 (6%)
2	JDP	K	901	-	33,35,35	2.18	6 (18%)	32,50,50	3.13	7 (21%)
3	ADP	D	902	-	24,29,29	0.88	0	29,45,45	1.16	2 (6%)
2	JDP	D	901	-	33,35,35	2.18	6 (18%)	32,50,50	3.13	7 (21%)
2	JDP	H	901	-	33,35,35	2.18	6 (18%)	32,50,50	3.12	7 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	ADP	H	902	-	24,29,29	0.88	0	29,45,45	1.16	2 (6%)
2	JDP	L	901	-	33,35,35	2.18	6 (18%)	32,50,50	3.12	7 (21%)
2	JDP	G	901	-	33,35,35	2.18	6 (18%)	32,50,50	3.12	7 (21%)
3	ADP	J	902	-	24,29,29	0.86	0	29,45,45	1.16	2 (6%)
3	ADP	C	902	-	24,29,29	0.87	0	29,45,45	1.17	2 (6%)
2	JDP	C	901	-	33,35,35	2.18	6 (18%)	32,50,50	3.12	7 (21%)

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	-	-	0/12/32/32	0/3/3/3
3	ADP	K	902	-	-	1/12/32/32	0/3/3/3
2	JDP	I	901	-	-	4/9/20/20	0/5/5/5
3	ADP	I	902	-	-	1/12/32/32	0/3/3/3
2	JDP	B	901	-	-	4/9/20/20	0/5/5/5
3	ADP	F	902	-	-	0/12/32/32	0/3/3/3
3	ADP	B	902	-	-	0/12/32/32	0/3/3/3
2	JDP	E	901	-	-	4/9/20/20	0/5/5/5
2	JDP	A	901	-	-	4/9/20/20	0/5/5/5
3	ADP	E	902	-	-	0/12/32/32	0/3/3/3
2	JDP	J	901	-	-	4/9/20/20	0/5/5/5
2	JDP	F	901	-	-	4/9/20/20	0/5/5/5
3	ADP	L	902	-	-	1/12/32/32	0/3/3/3
3	ADP	G	902	-	-	1/12/32/32	0/3/3/3
2	JDP	K	901	-	-	4/9/20/20	0/5/5/5
3	ADP	D	902	-	-	0/12/32/32	0/3/3/3
2	JDP	D	901	-	-	4/9/20/20	0/5/5/5
2	JDP	H	901	-	-	4/9/20/20	0/5/5/5
3	ADP	H	902	-	-	1/12/32/32	0/3/3/3
2	JDP	L	901	-	-	4/9/20/20	0/5/5/5
2	JDP	G	901	-	-	4/9/20/20	0/5/5/5
3	ADP	J	902	-	-	1/12/32/32	0/3/3/3
3	ADP	C	902	-	-	0/12/32/32	0/3/3/3
2	JDP	C	901	-	-	4/9/20/20	0/5/5/5

The worst 5 of 72 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	JDP	C15-N16	7.06	1.45	1.34
2	B	901	JDP	C15-N16	7.05	1.45	1.34
2	H	901	JDP	C15-N16	7.05	1.45	1.34
2	G	901	JDP	C15-N16	7.03	1.45	1.34
2	C	901	JDP	C15-N16	7.02	1.45	1.34

The worst 5 of 109 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	901	JDP	C11-C10-C09	-15.42	100.95	128.71
2	A	901	JDP	C11-C10-C09	-15.41	100.95	128.71
2	E	901	JDP	C11-C10-C09	-15.39	100.99	128.71
2	C	901	JDP	C11-C10-C09	-15.39	100.99	128.71
2	K	901	JDP	C11-C10-C09	-15.39	100.99	128.71

There are no chirality outliers.

5 of 54 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	901	JDP	N14-C15-N16-C17
2	A	901	JDP	C24-C15-N16-C17
2	B	901	JDP	N14-C15-N16-C17
2	B	901	JDP	C24-C15-N16-C17
2	C	901	JDP	N14-C15-N16-C17

There are no ring outliers.

21 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	902	ADP	2	0
3	K	902	ADP	1	0
2	I	901	JDP	1	0
3	I	902	ADP	2	0
2	B	901	JDP	1	0
3	F	902	ADP	3	0
2	E	901	JDP	1	0
2	A	901	JDP	1	0
2	J	901	JDP	1	0
2	F	901	JDP	1	0
3	L	902	ADP	3	0

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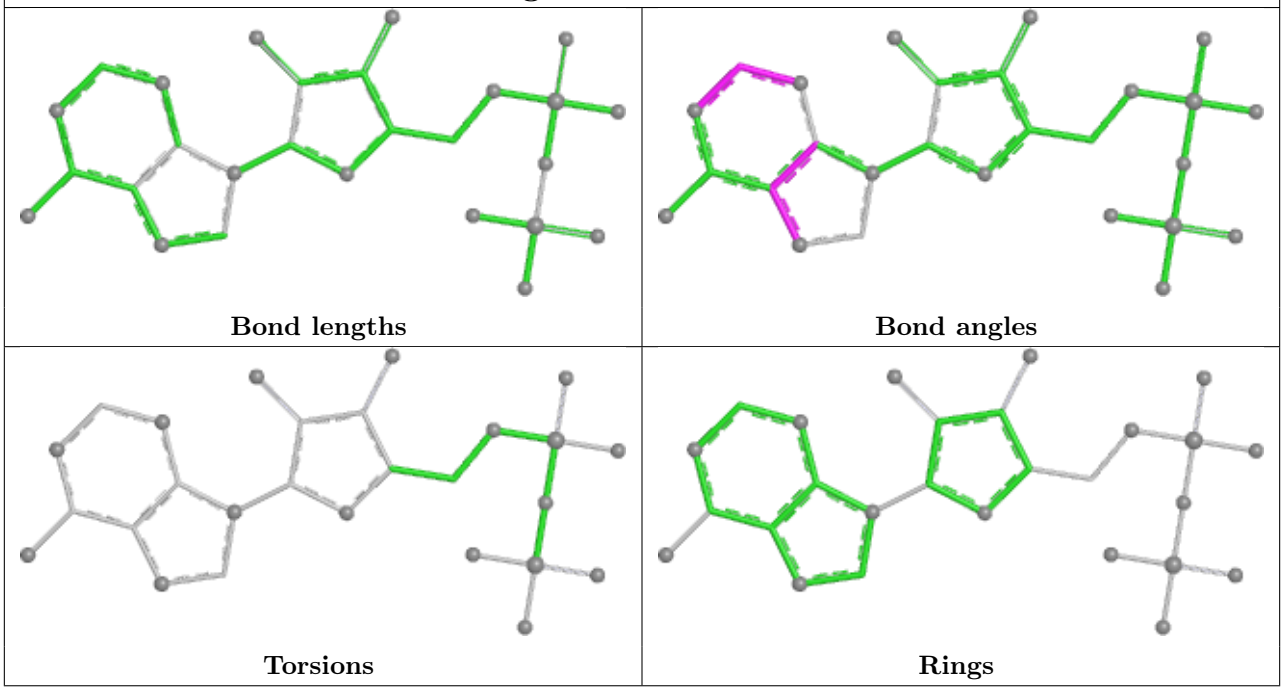
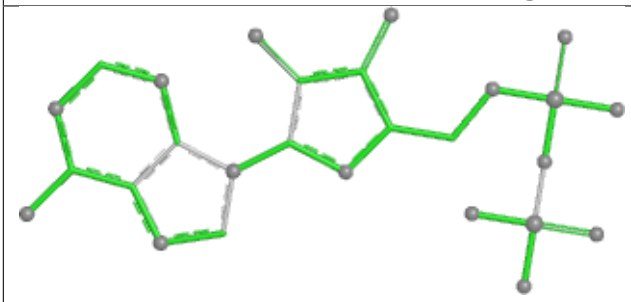
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	902	ADP	3	0
2	K	901	JDP	1	0
3	D	902	ADP	1	0
2	D	901	JDP	1	0
2	H	901	JDP	2	0
3	H	902	ADP	1	0
2	L	901	JDP	1	0
2	G	901	JDP	1	0
3	C	902	ADP	1	0
2	C	901	JDP	1	0

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 ADP A 902



Ligand ADP K 902



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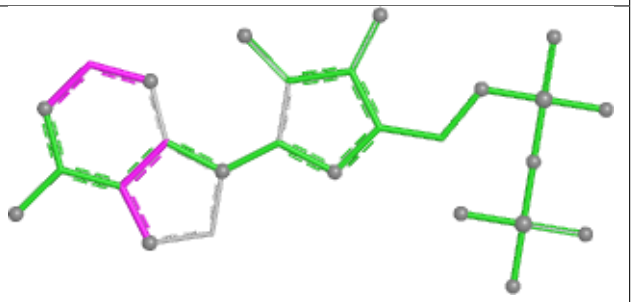
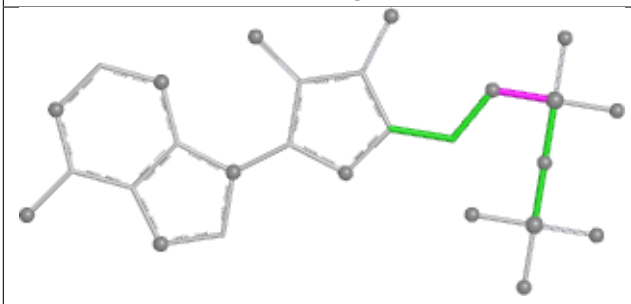
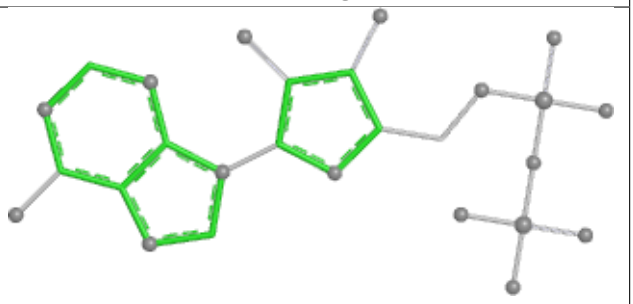


Bond angles

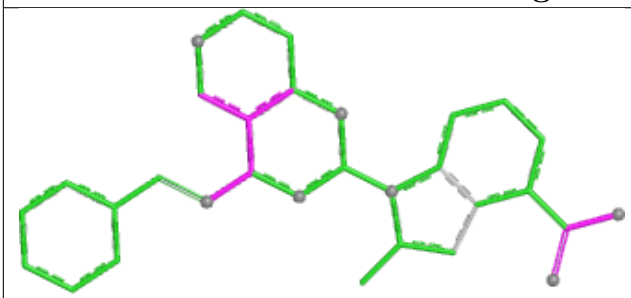


Torsions



Rings

Ligand JDP I 901



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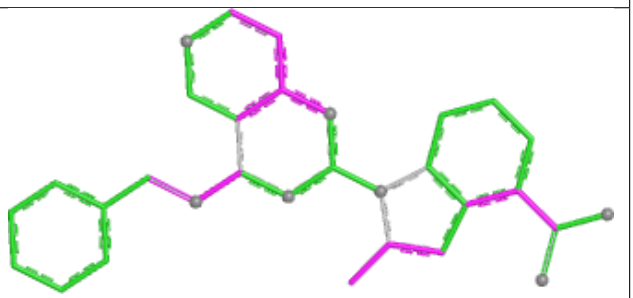

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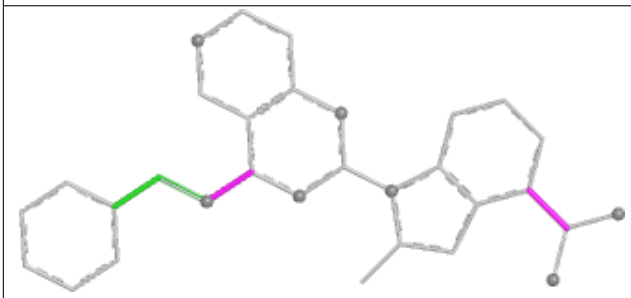

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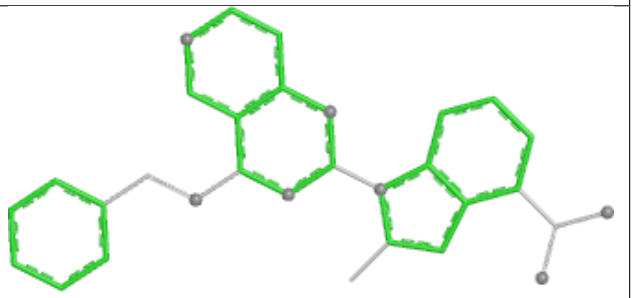

Rings

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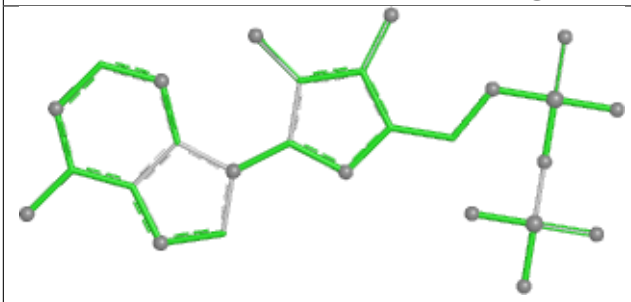

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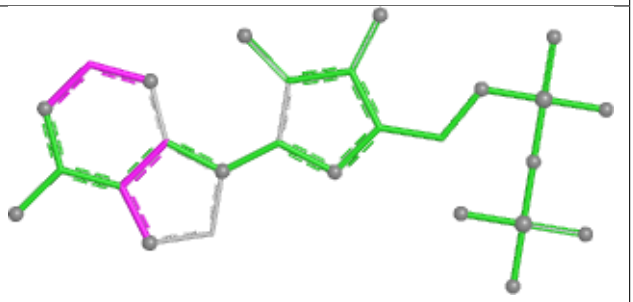

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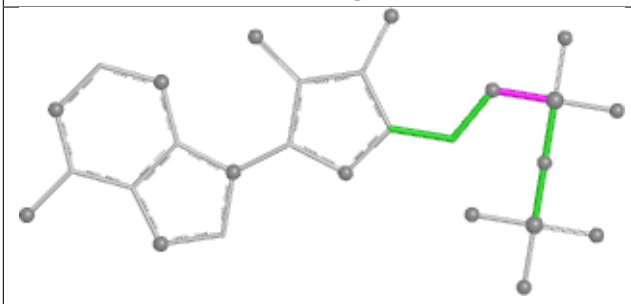

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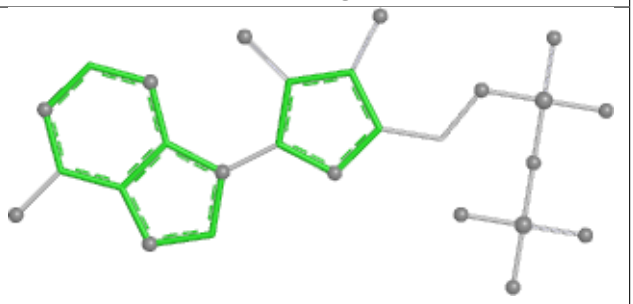
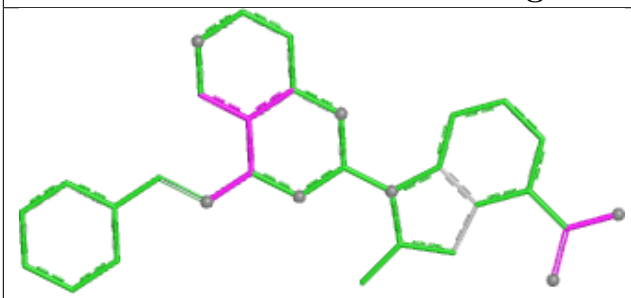


Rings

Ligand JDP B 901



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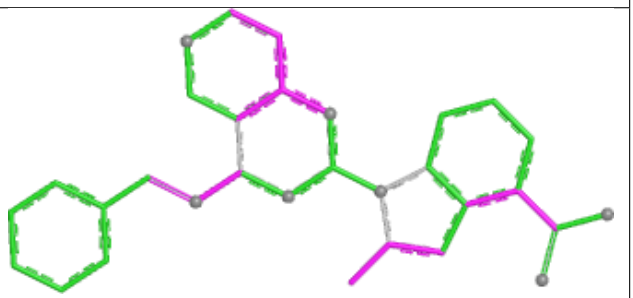

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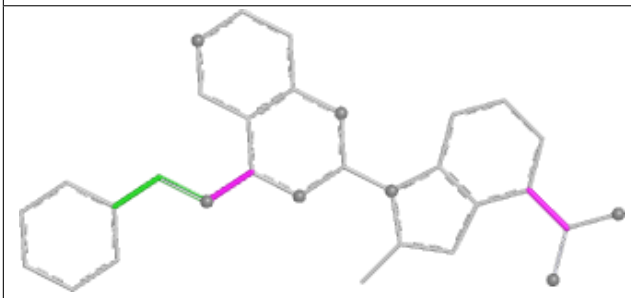

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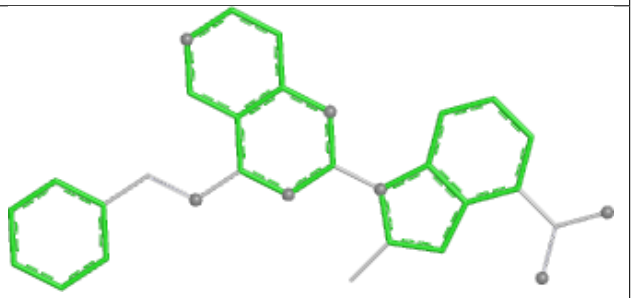
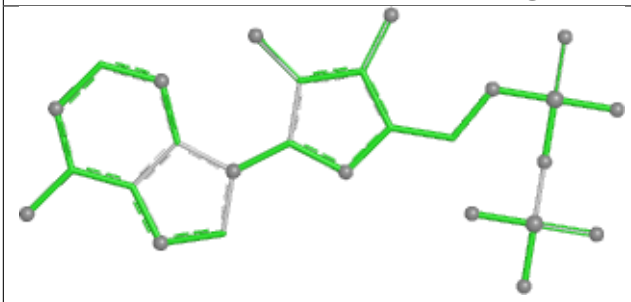


Rings

Ligand ADP F 902



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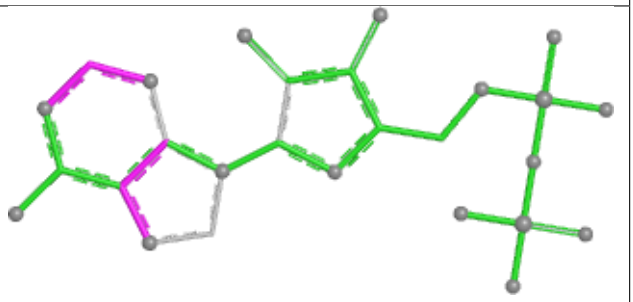

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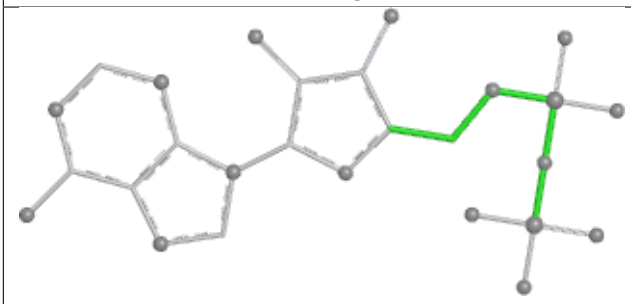

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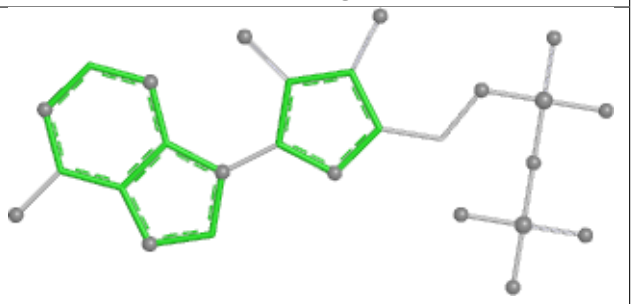

Rings

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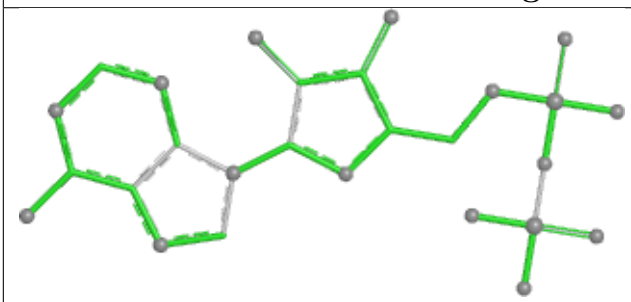

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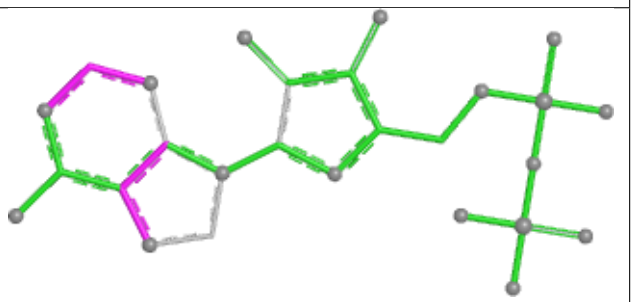

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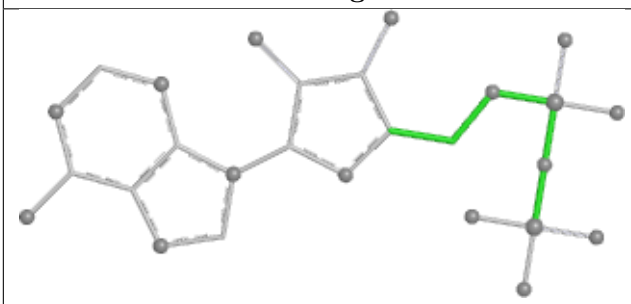

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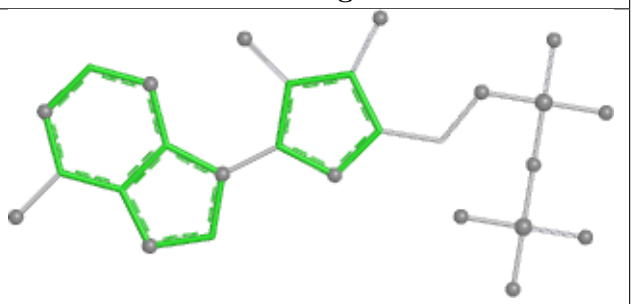
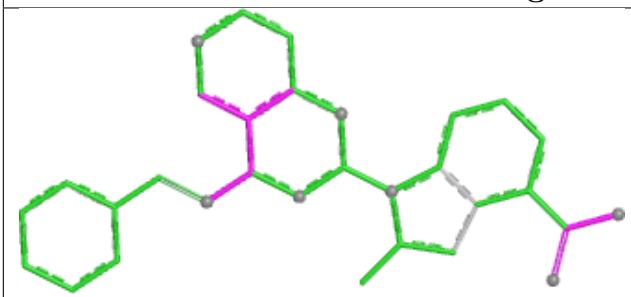


Rings

Ligand JDP E 901



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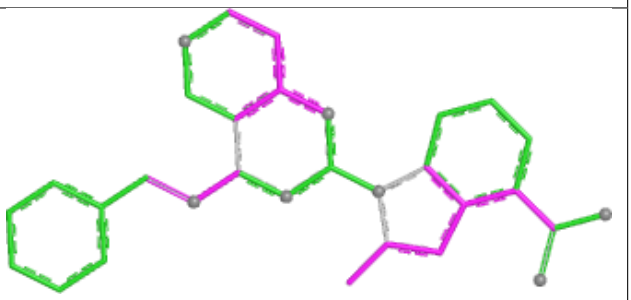

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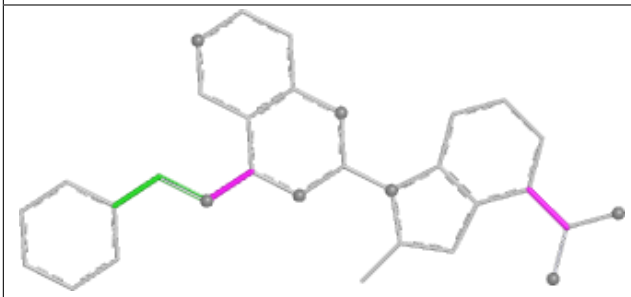

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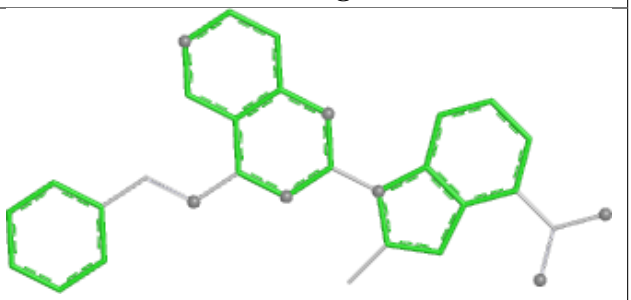

Rings

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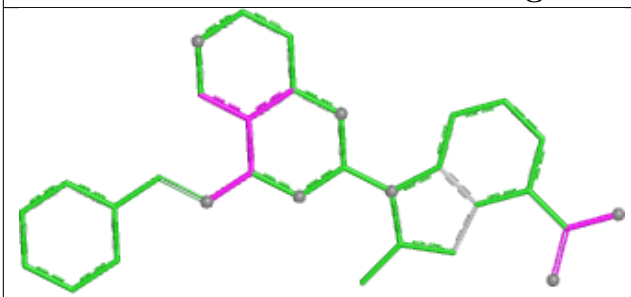

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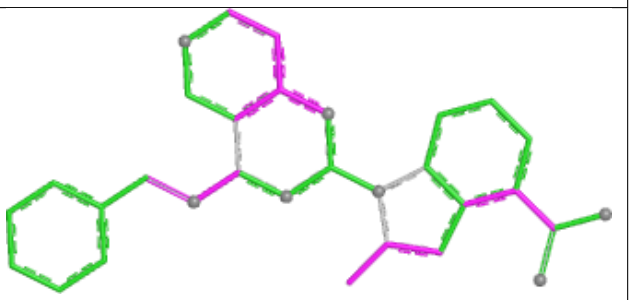

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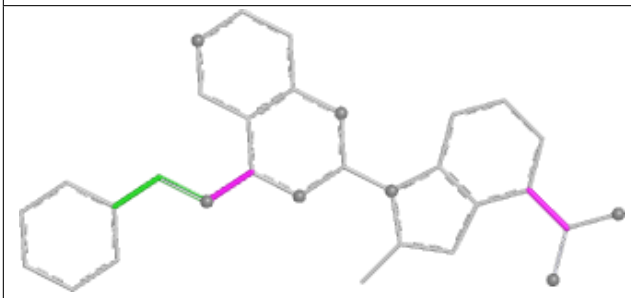

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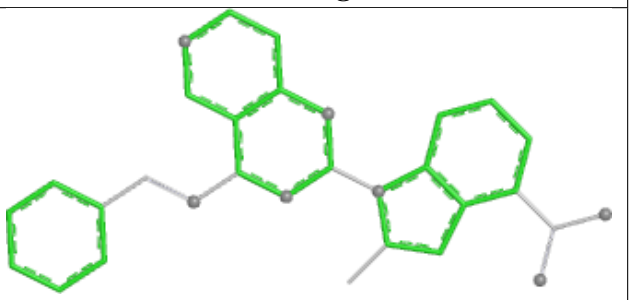
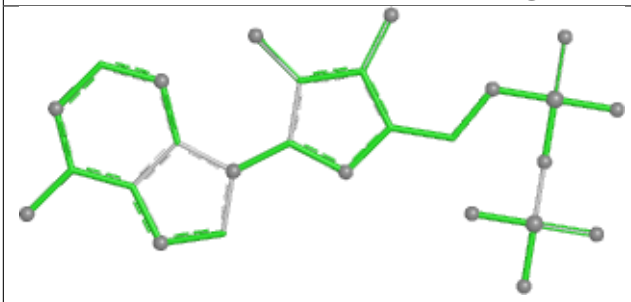


Rings

Ligand ADP E 902



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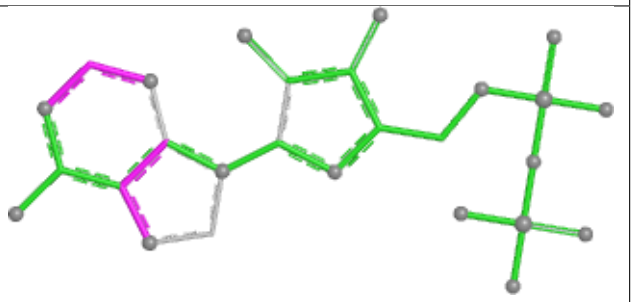

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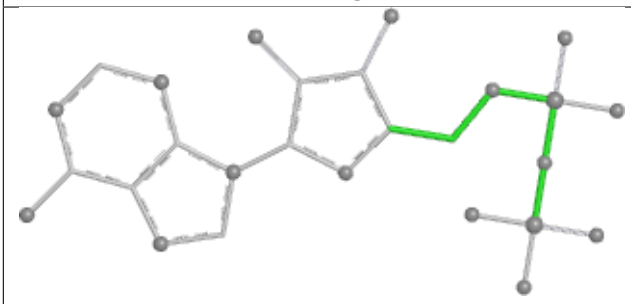

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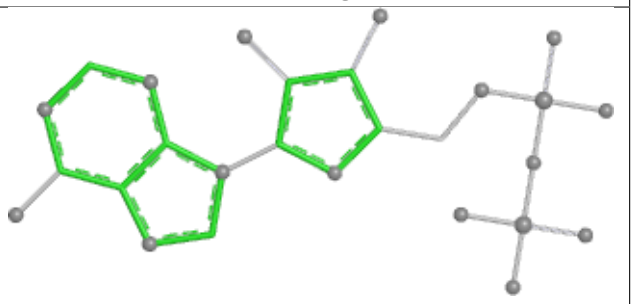
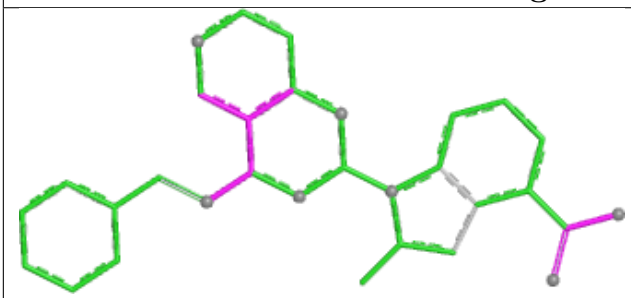


Rings

Ligand JDP J 901



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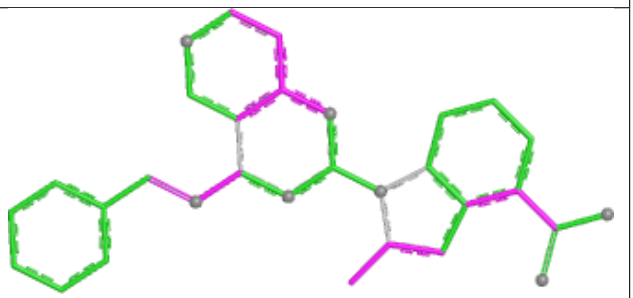
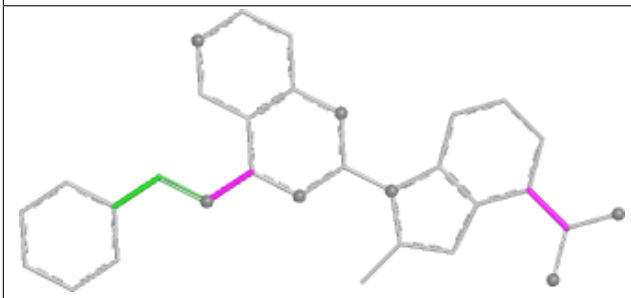
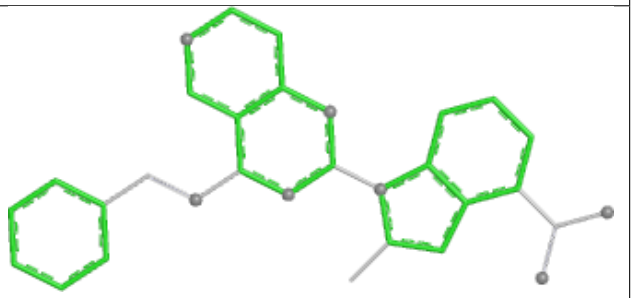


Bond angles



Torsions



Rings

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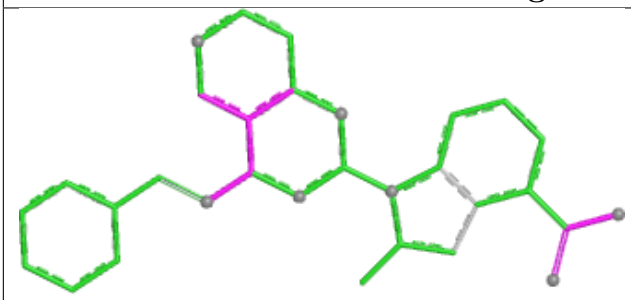

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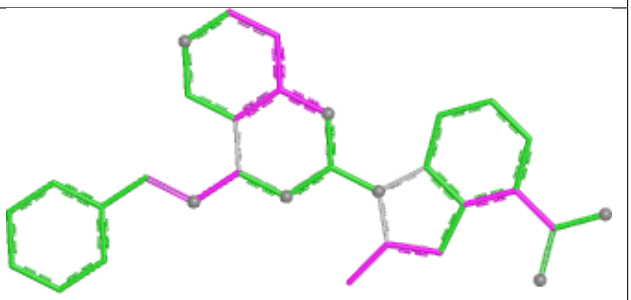

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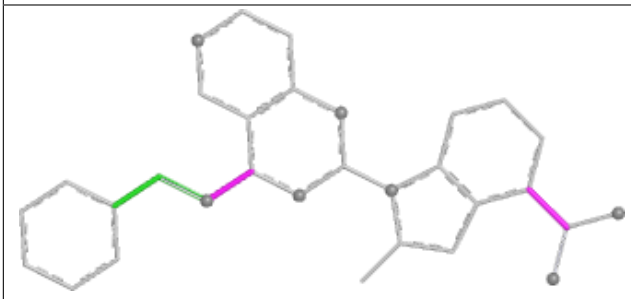
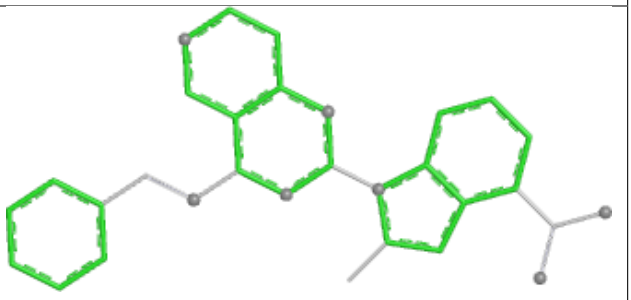
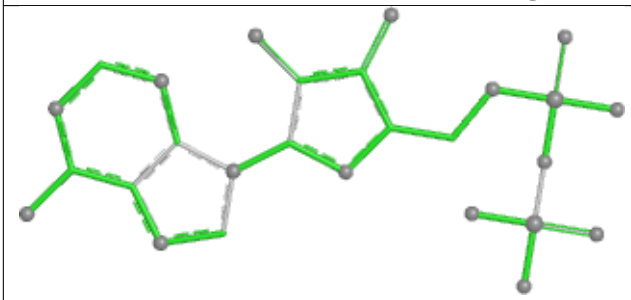


Torsions

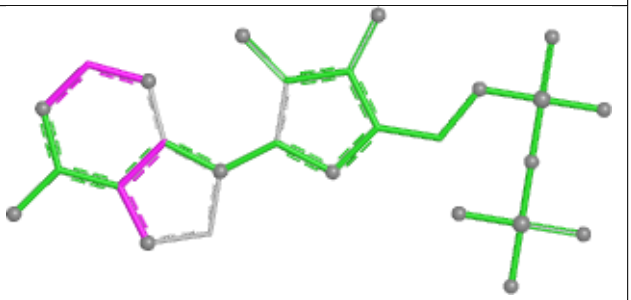


Rings

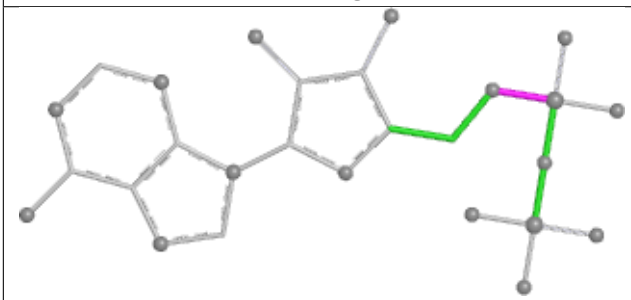
Ligand ADP L 902



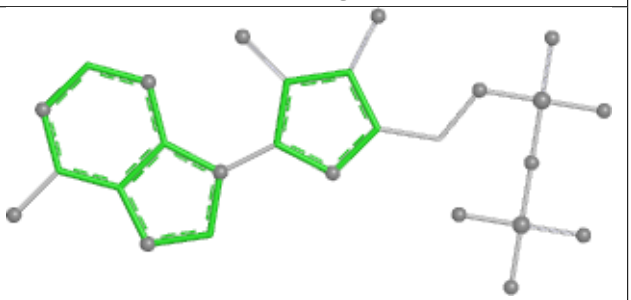
Bond lengths



Bond angles

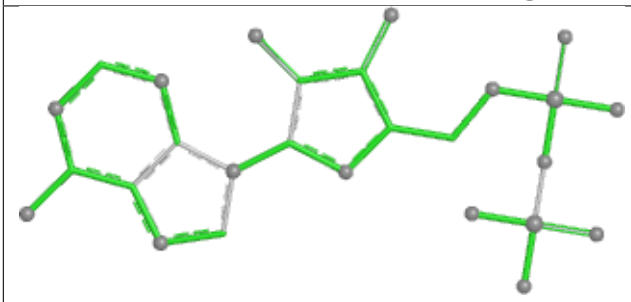


Torsions



Rings

Ligand ADP G 902



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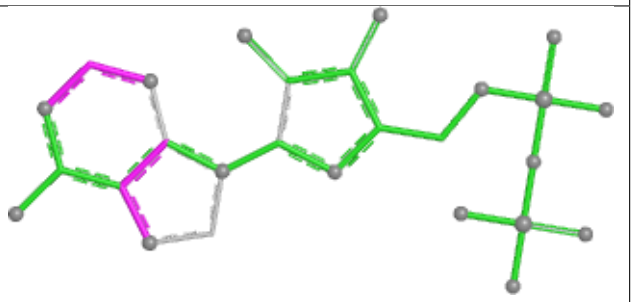
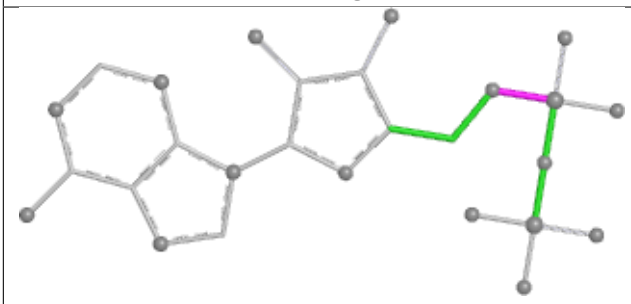
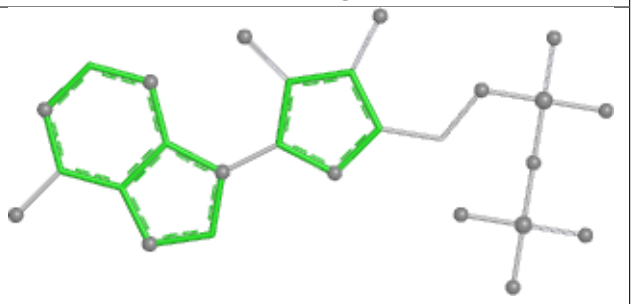


Bond angles

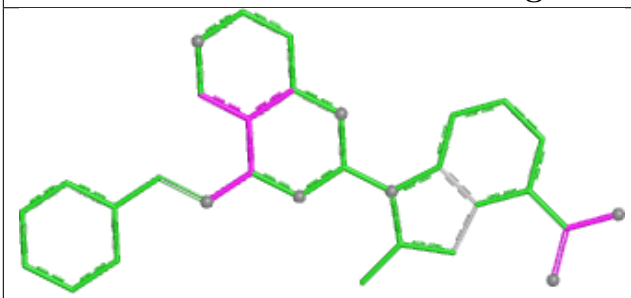


Torsions

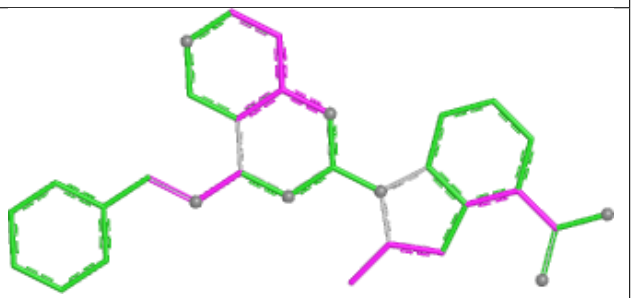


Rings

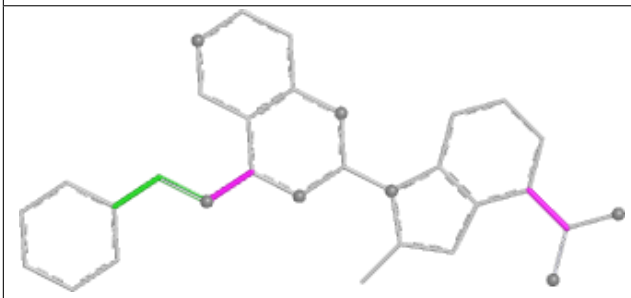
Ligand JDP K 901



Bond lengths



Bond angles



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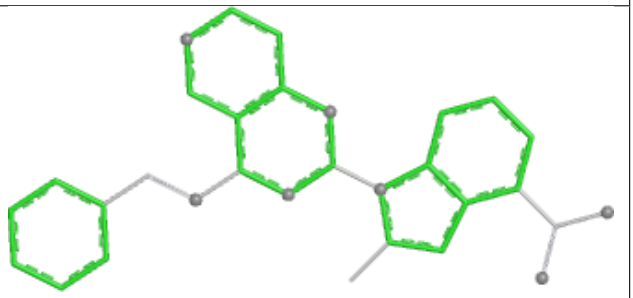
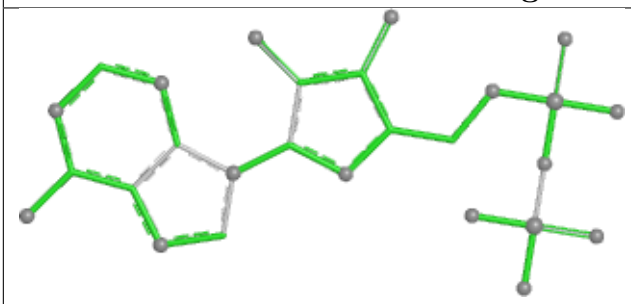
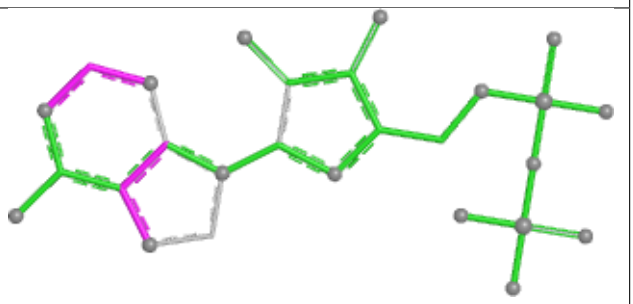


Rings

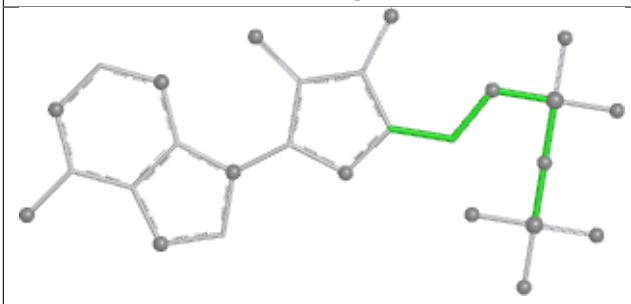
Ligand ADP D 902



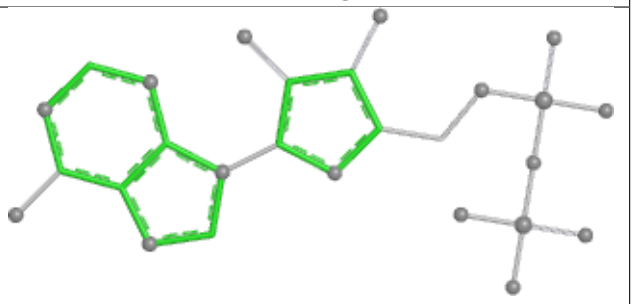
Bond lengths



Bond angles

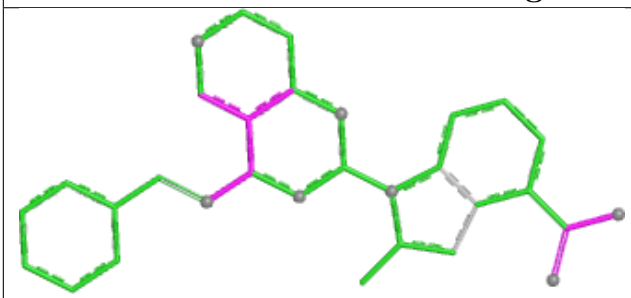


Torsions

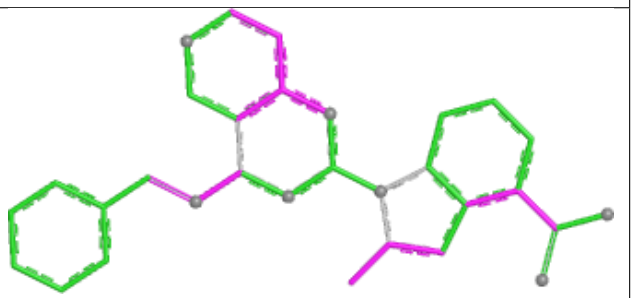


Rings

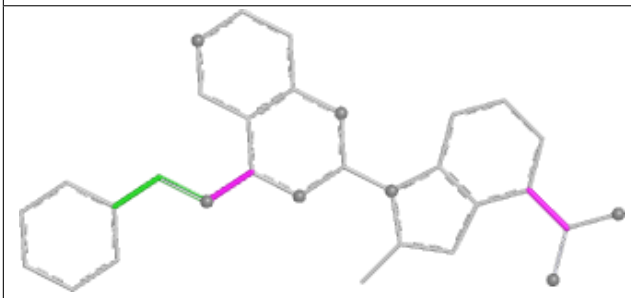
Ligand JDP D 901



Bond lengths



Bond angles



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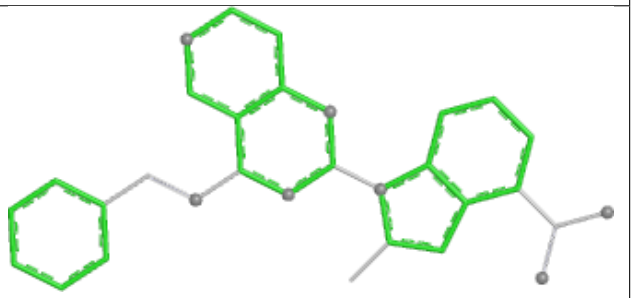
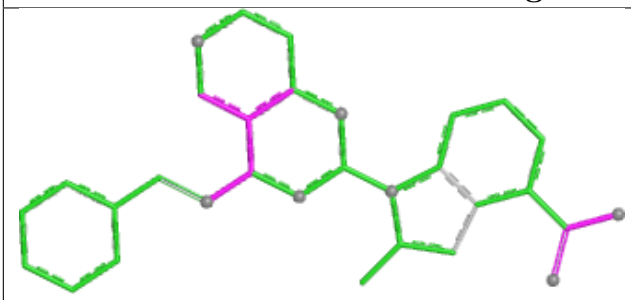


Rings

Ligand JDP H 901



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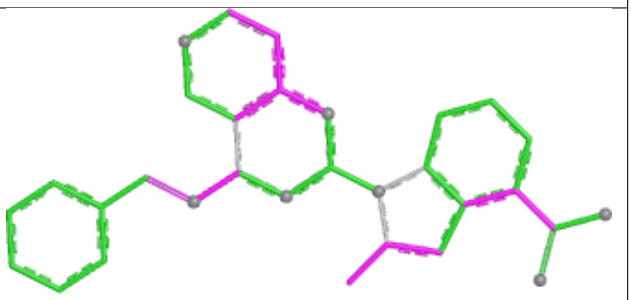
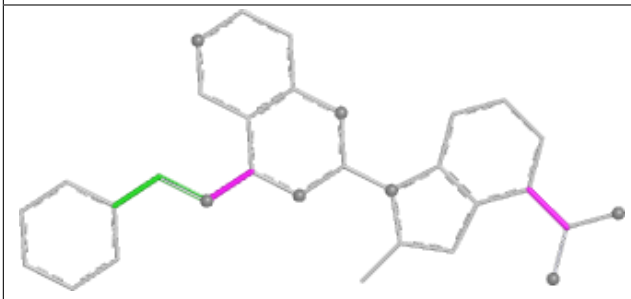
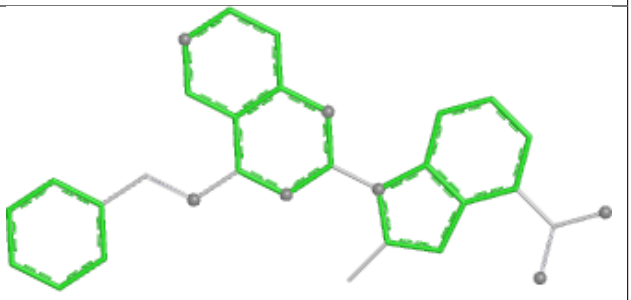


Bond angles

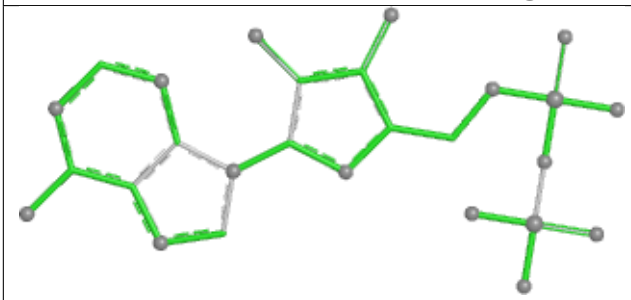


Torsions



Rings

Ligand ADP H 902



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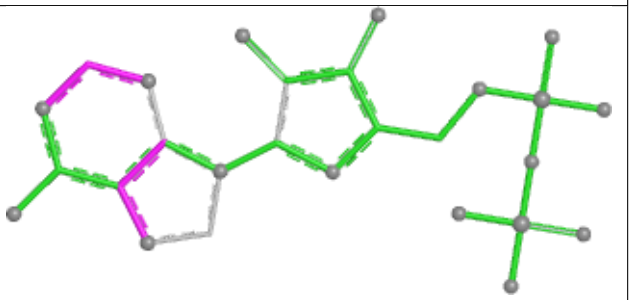
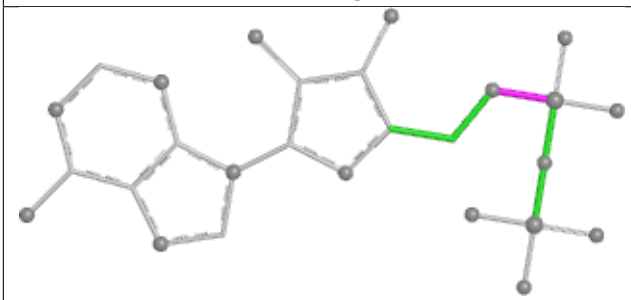
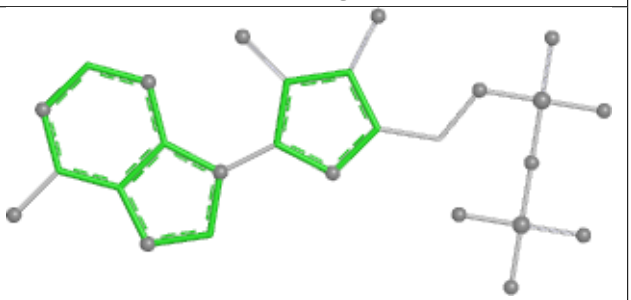


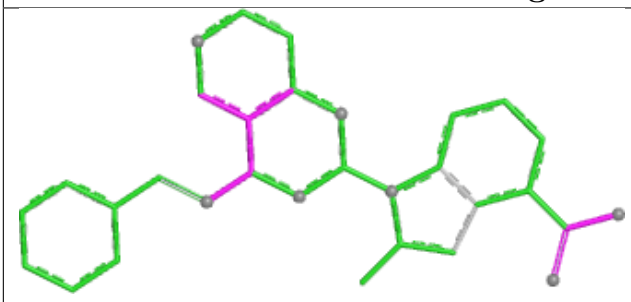
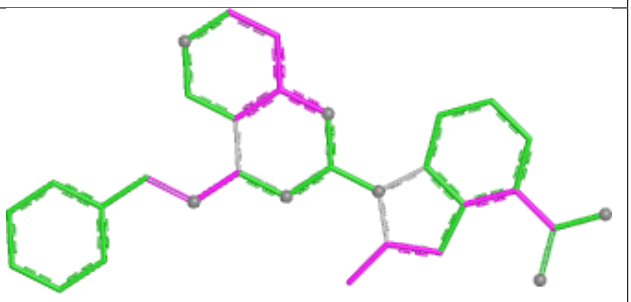
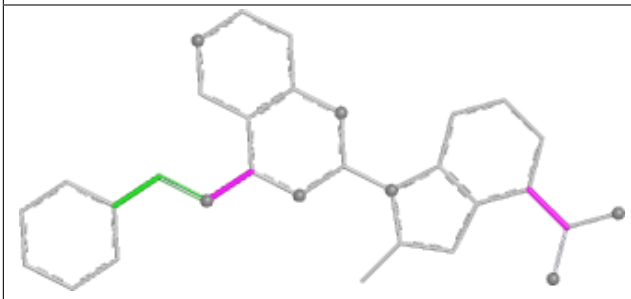
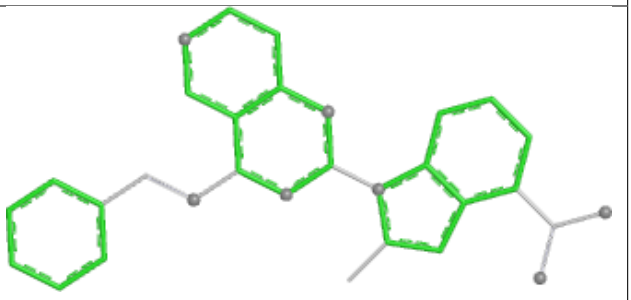
Bond angles

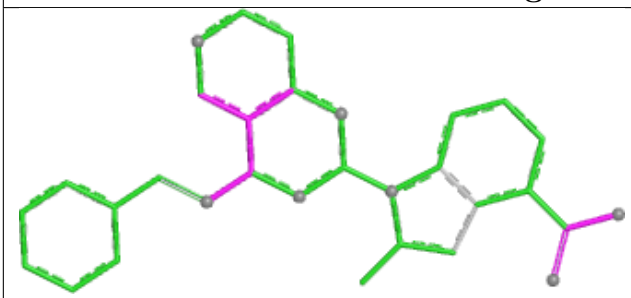
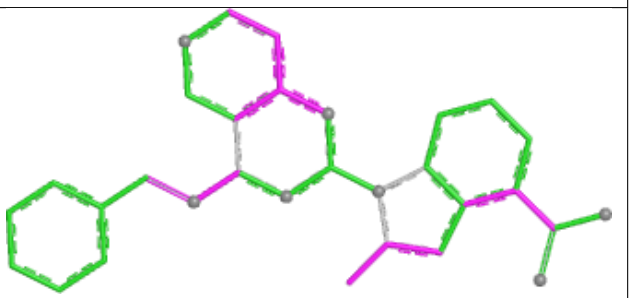
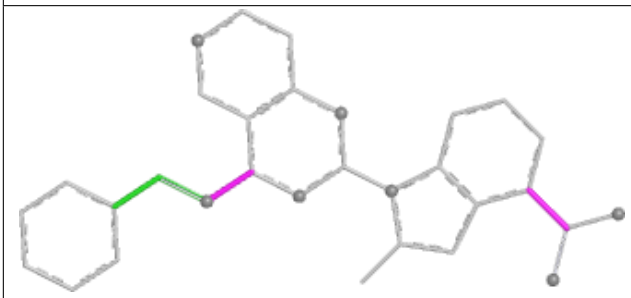
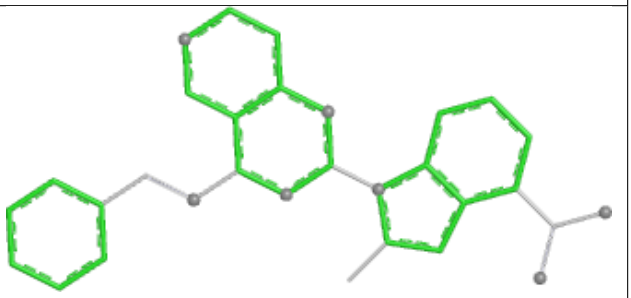


Torsions

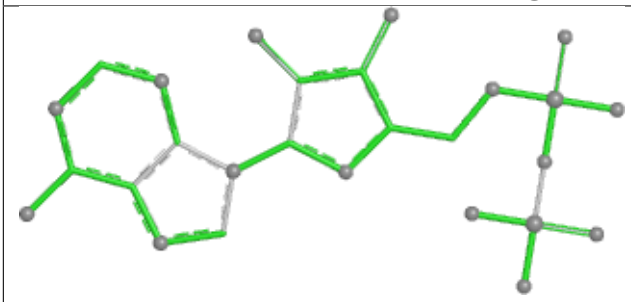


Rings

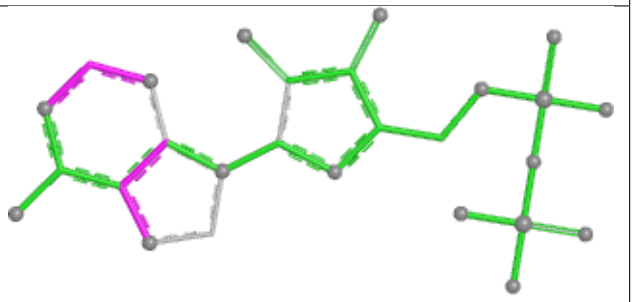
Ligand JDP L 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand JDP G 901	
 Bond lengths	 Bond angles
 Torsions	 Rings

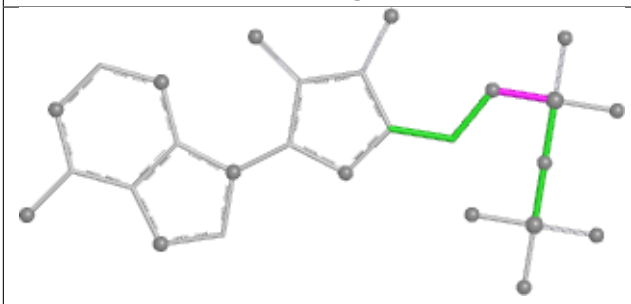
Ligand ADP J 902



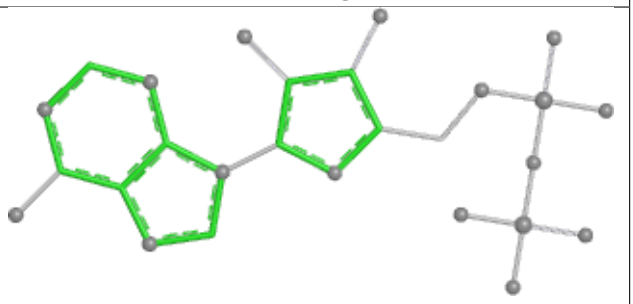
Bond lengths



Bond angles

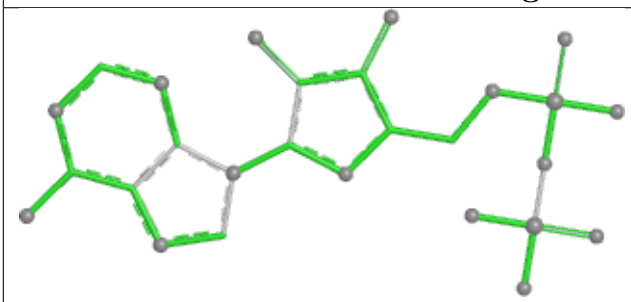


Torsions

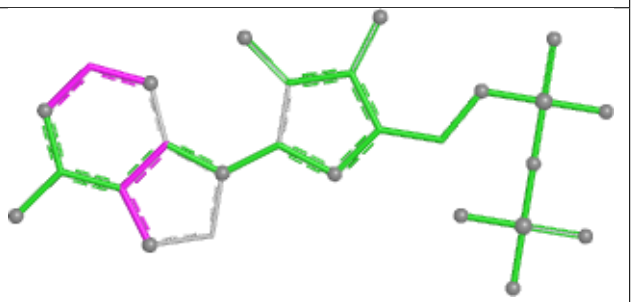


Rings

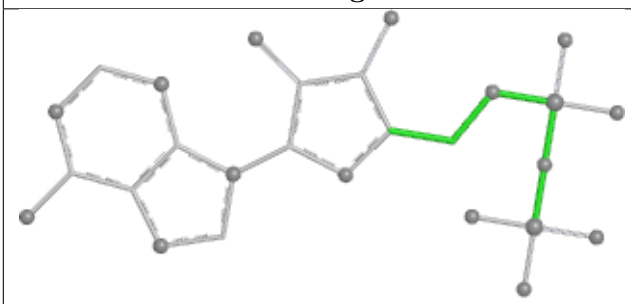
Ligand ADP C 902



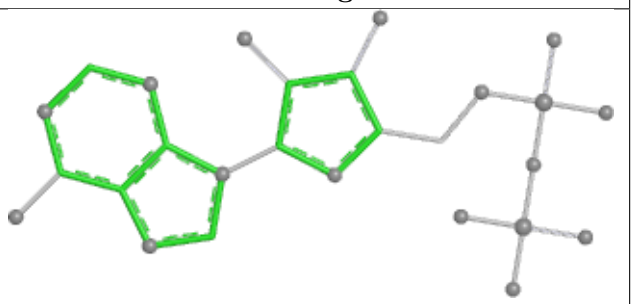
Bond lengths



Bond angles

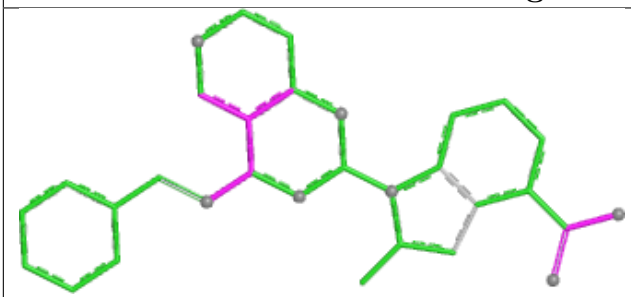


Torsions

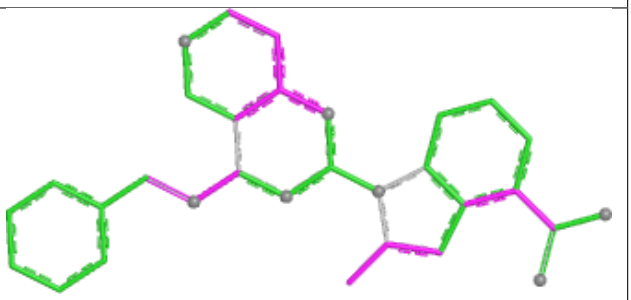


Rings

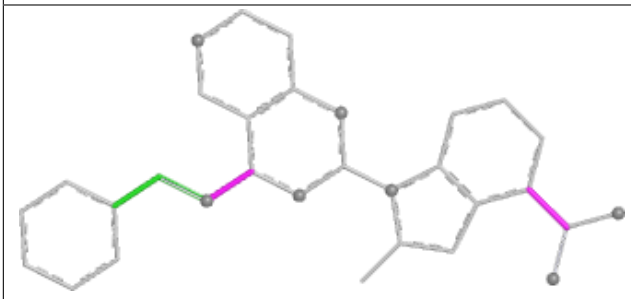
Ligand JDP C 901



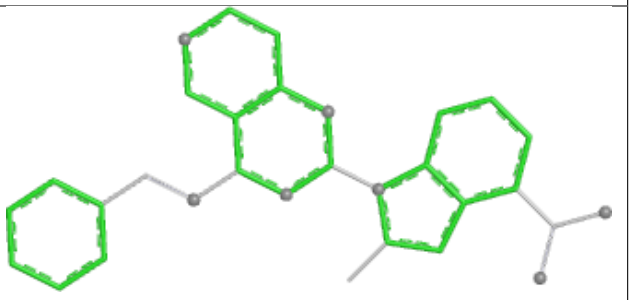
Bond lengths



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.

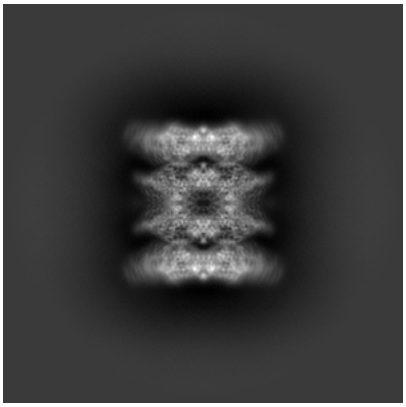
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24531. These allow visual inspection of the internal detail of the map and identification of artifacts.

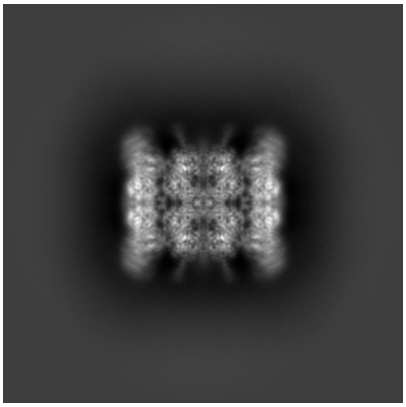
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

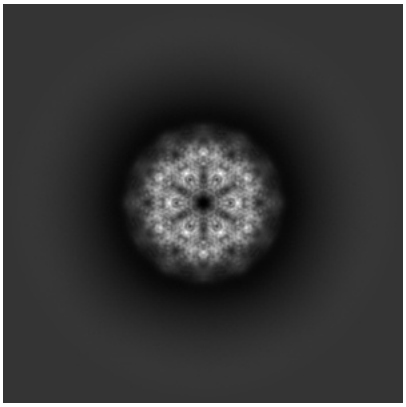
6.1.1 Primary map



X



Y

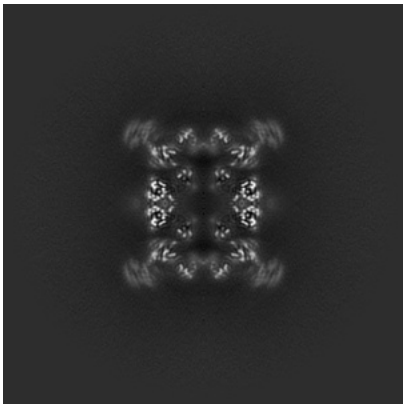


Z

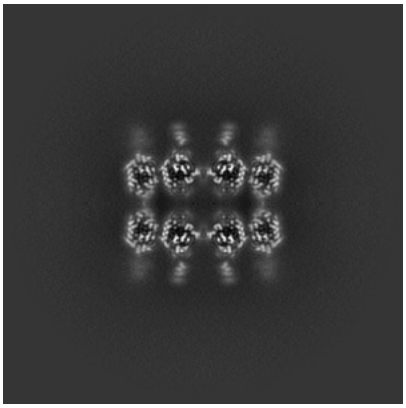
The images above show the map projected in three orthogonal directions.

6.2 Central slices

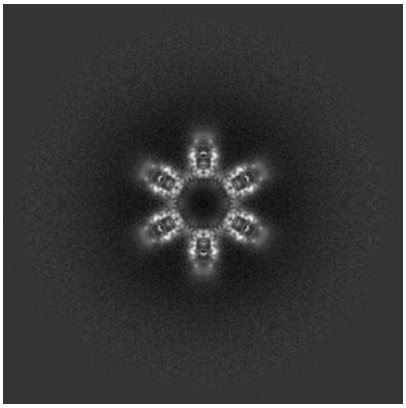
6.2.1 Primary map



X Index: 200



Y Index: 200

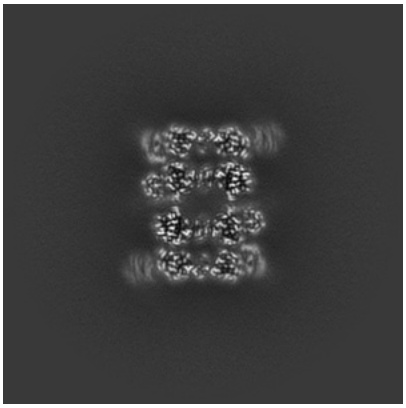


Z Index: 200

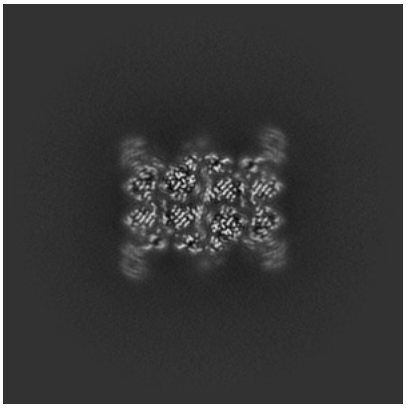
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

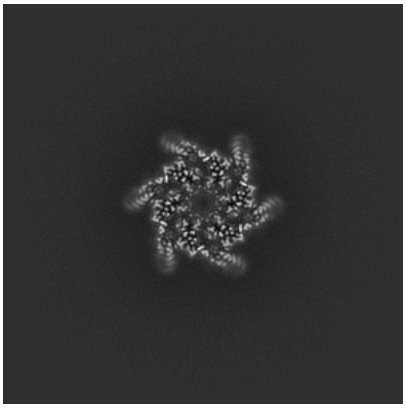
6.3.1 Primary map



X Index: 185



Y Index: 171

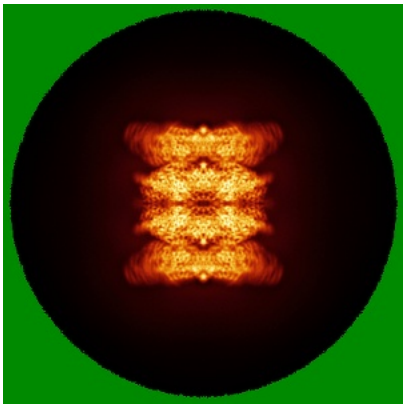


Z Index: 179

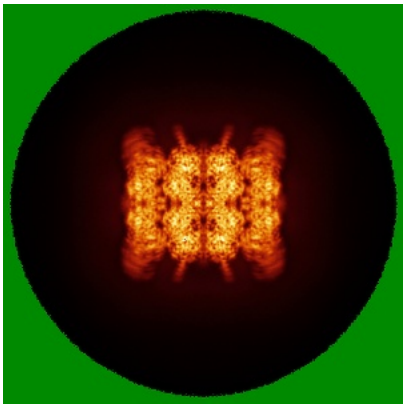
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

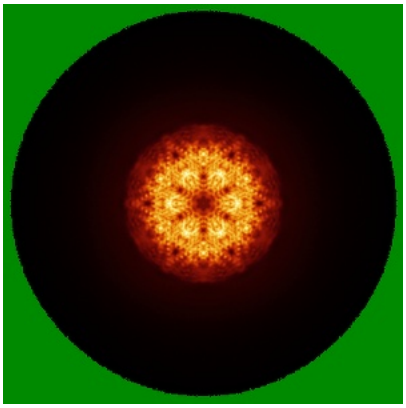
6.4.1 Primary map



X



Y

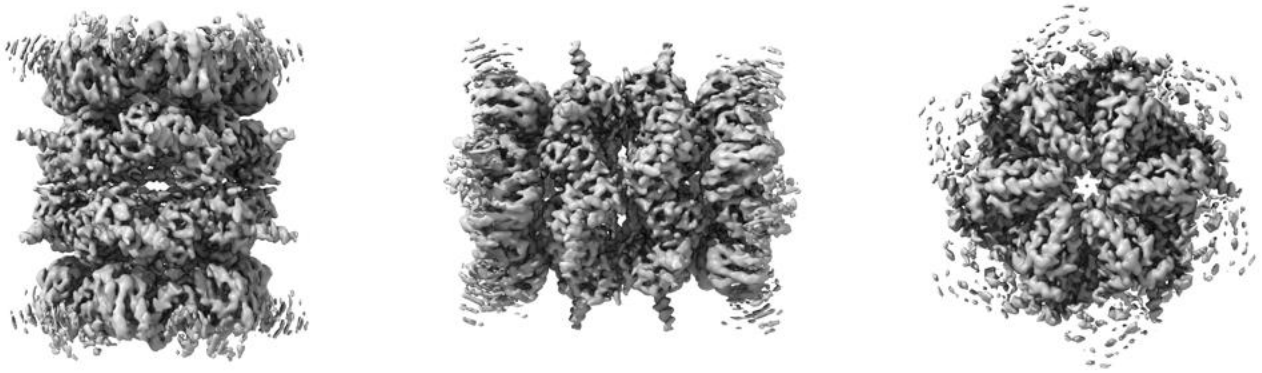


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

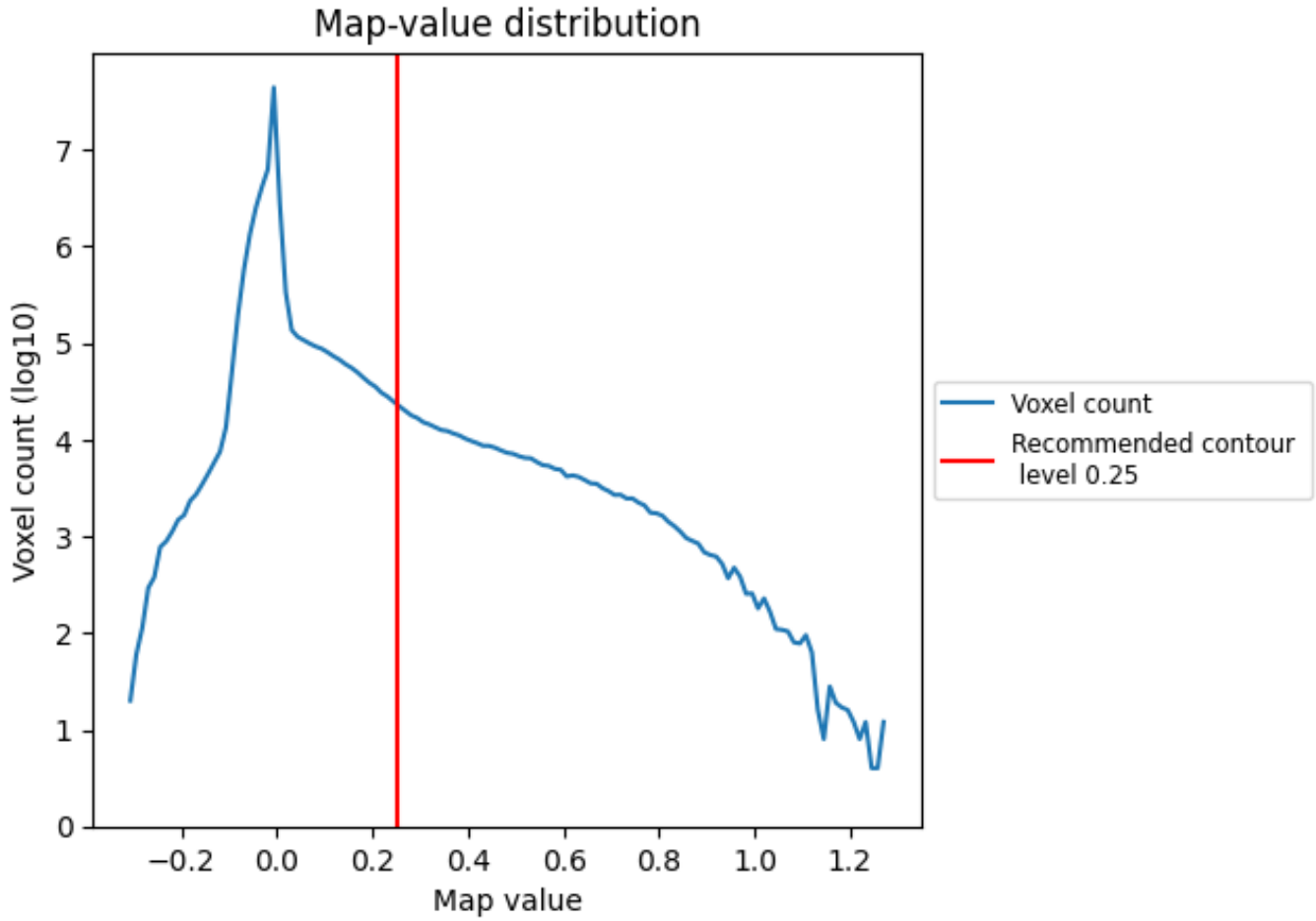
6.6 Mask visualisation (i)

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

7 Map analysis

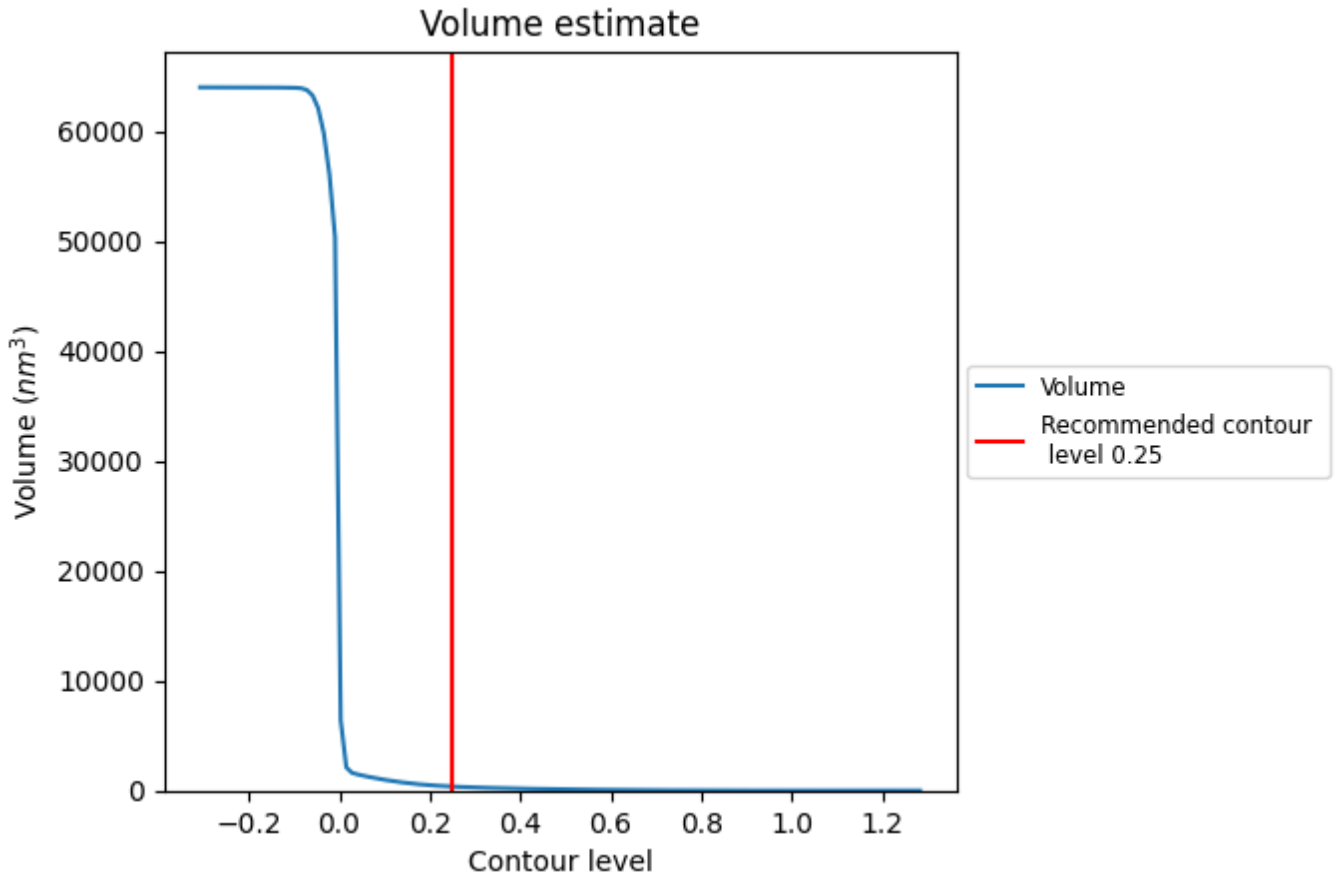
This section contains the results of statistical analysis of the map.

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.

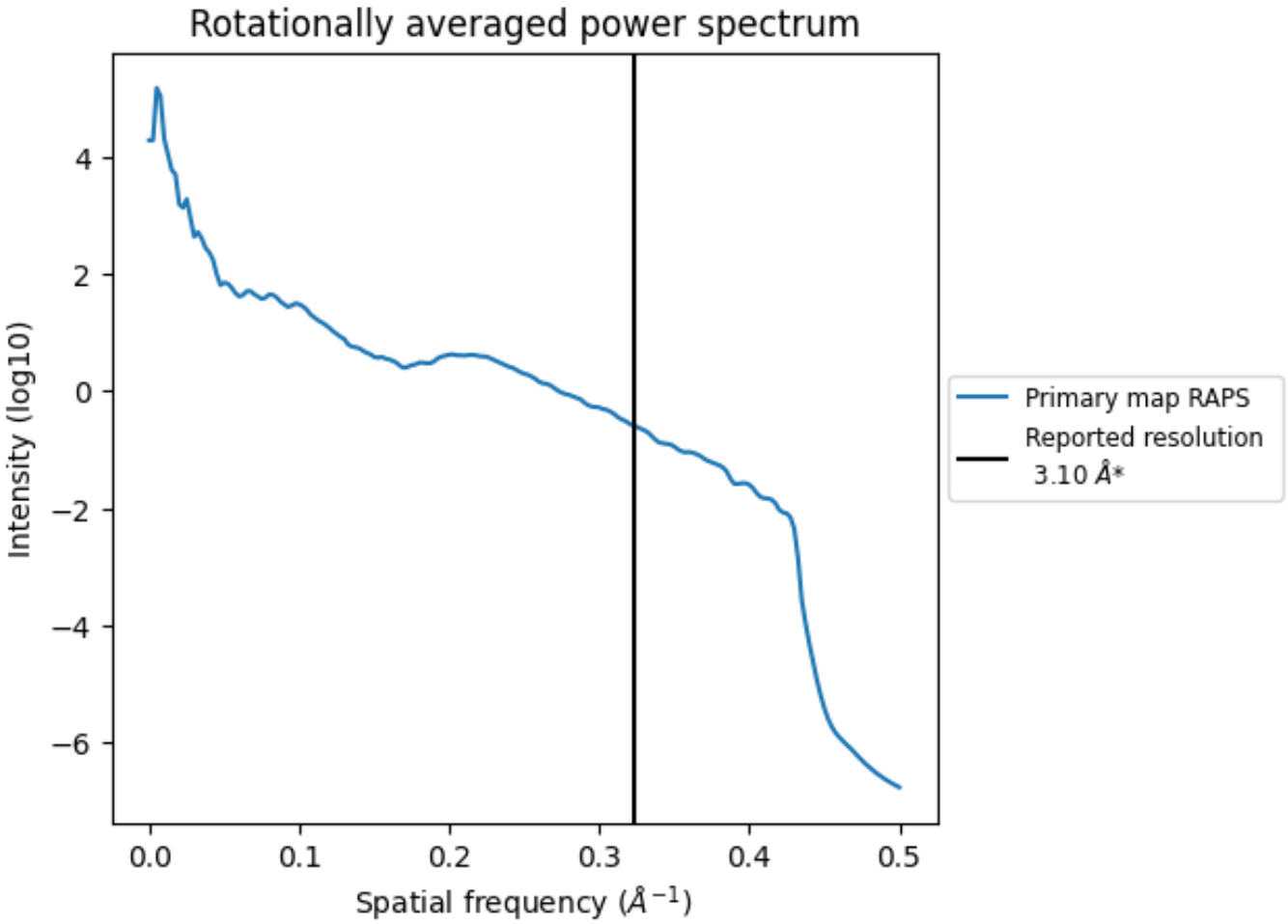
7.2 Volume estimate (i)



The volume at the recommended contour level is 364 nm^3; this corresponds to an approximate mass of 329 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)

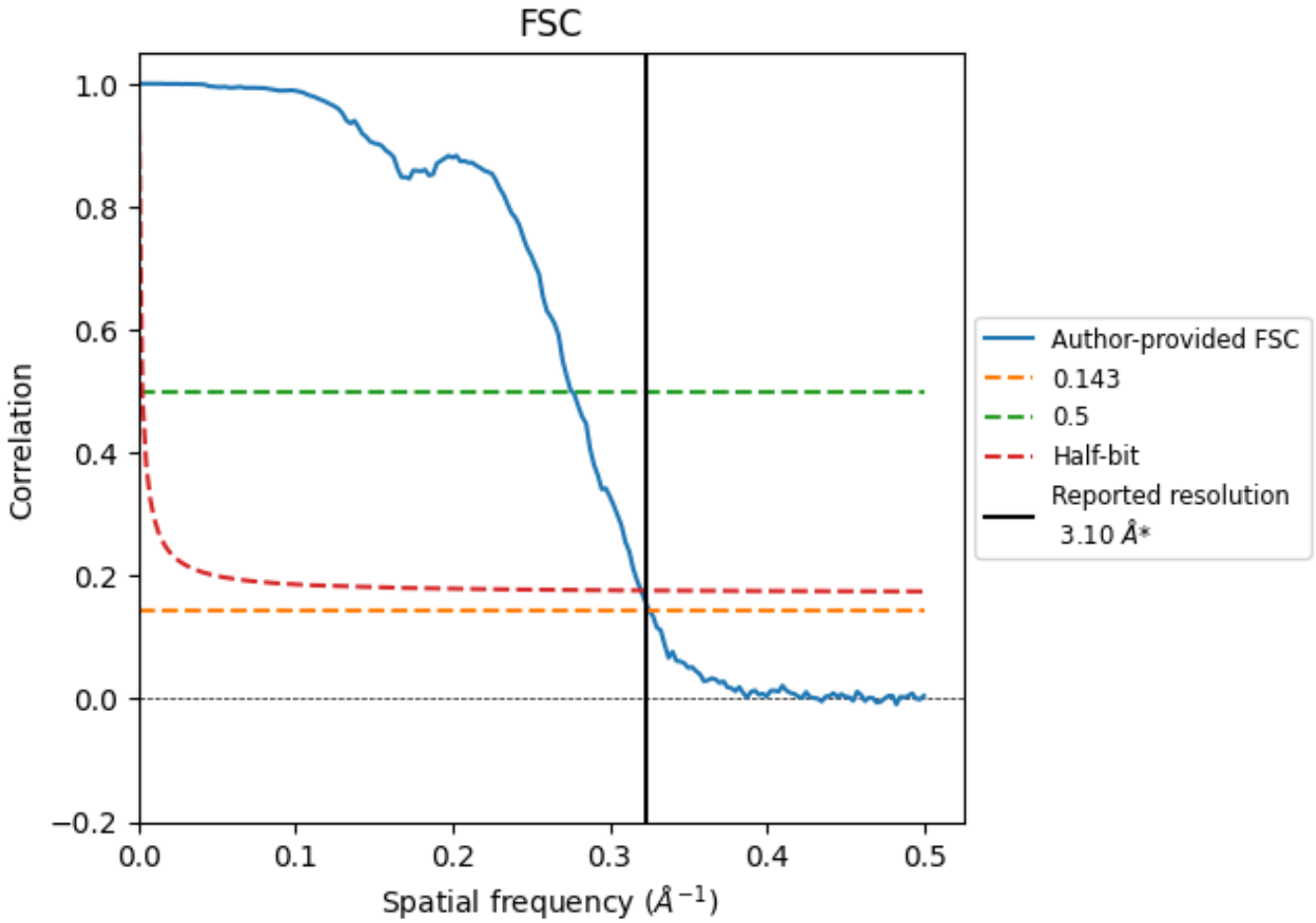


*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.323 Å^{-1}

8.2 Resolution estimates (i)

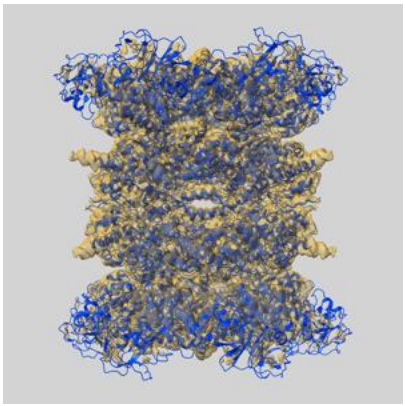
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.10	-	-
Author-provided FSC curve	3.08	3.62	3.13
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

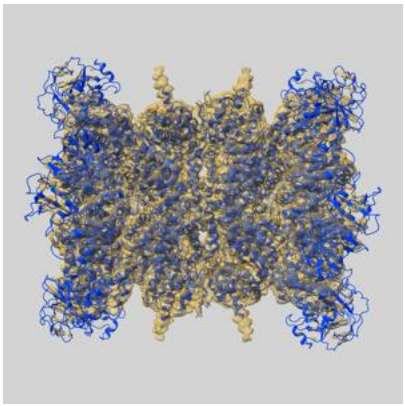
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-24531 and PDB model 7RLI. Per-residue inclusion information can be found in section 3 on page 12.

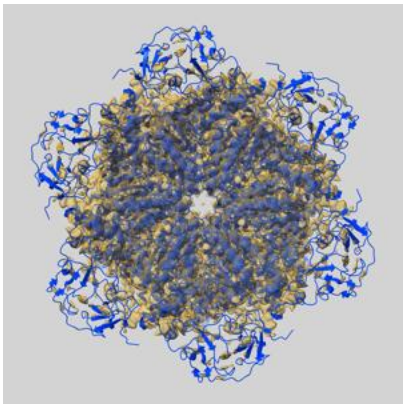
9.1 Map-model overlay



X



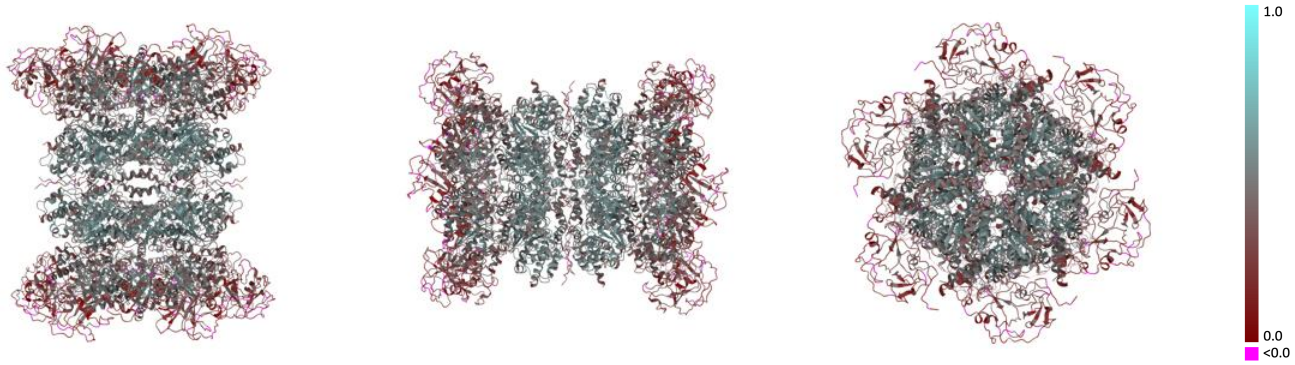
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

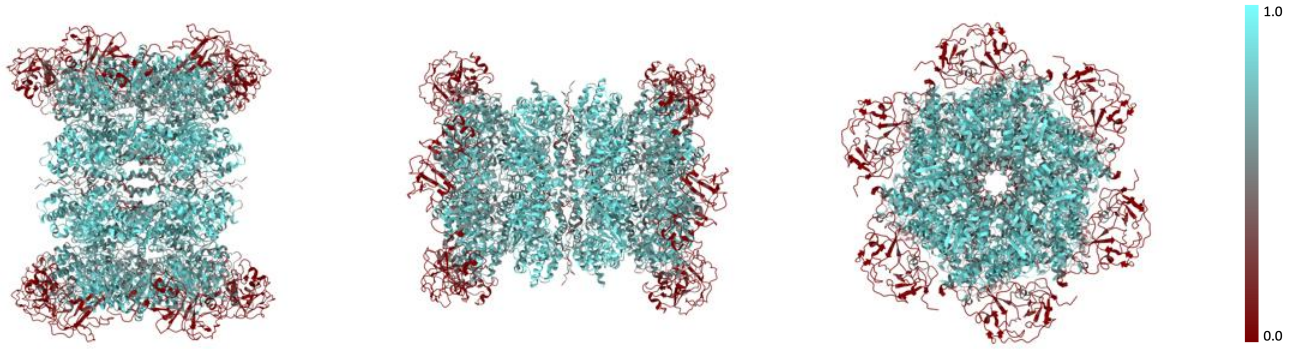
9.2 Q-score mapped to coordinate model (i)



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.

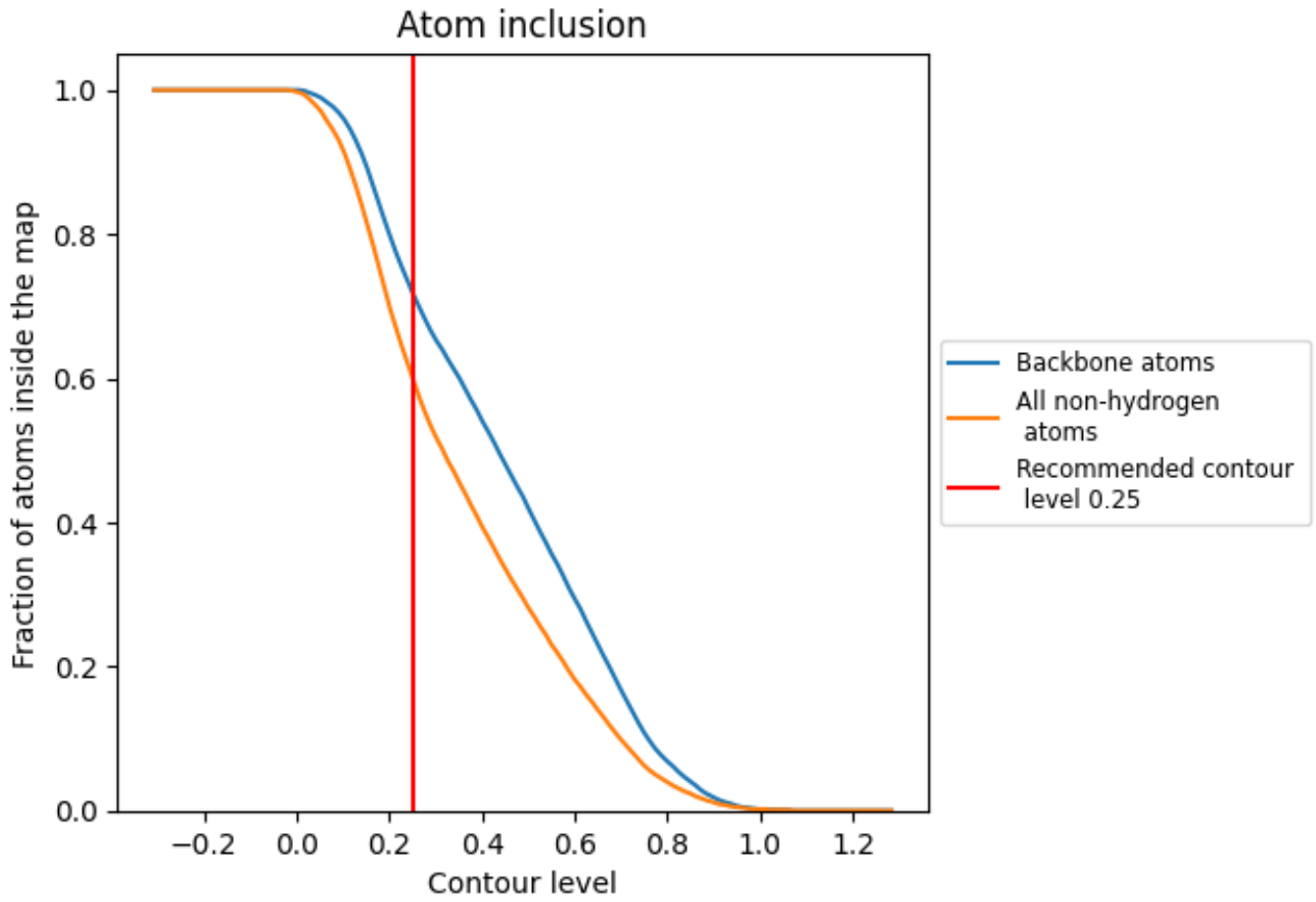
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 60% 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 (0.25) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6000	0.3930
A	0.6010	0.3940
B	0.6000	0.3950
C	0.6000	0.3940
D	0.5990	0.3930
E	0.6000	0.3920
F	0.5990	0.3970
G	0.6000	0.3950
H	0.5990	0.3870
I	0.5990	0.3900
J	0.6000	0.3910
K	0.5990	0.3980
L	0.6010	0.3920