wwPDB EM Validation Summary Report (i)

Nov 7, 2022 – 03:12 AM EST

PDB ID	:	6C3P
EMDB ID	:	EMD-7339
Title	:	Cryo-EM structure of human KATP bound to ATP and ADP in propeller form
Authors	:	Lee, K.P.K.; Chen, J.; MacKinnon, R.
Deposited on	:	2018-01-10
Resolution	:	5.60 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 (1)) were used in the production of this report:

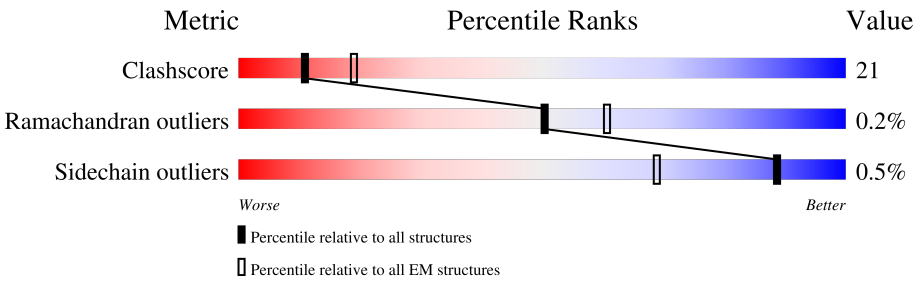
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 5.60 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	406	47% 34% 19%
1	B	406	45% 36% 19%
1	C	406	47% 34% 19%
1	D	406	47% 34% 19%
2	E	1581	53% 33% 14%
2	F	1581	53% 32% 14%
2	G	1581	5% 53% 32% 14%
2	H	1581	53% 32% 14%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 50696 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 ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	328	2506	1619	428	442	17	0	0
1	D	328	2506	1619	428	442	17	0	0
1	B	328	2506	1619	428	442	17	0	0
1	C	328	2506	1619	428	442	17	0	0

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	SER	-	expression tag	UNP Q14654
A	-4	ALA	-	expression tag	UNP Q14654
A	-3	SER	-	expression tag	UNP Q14654
A	-2	ALA	-	expression tag	UNP Q14654
A	-1	SER	-	expression tag	UNP Q14654
A	0	ALA	-	expression tag	UNP Q14654
A	391	SER	-	expression tag	UNP Q14654
A	392	ASN	-	expression tag	UNP Q14654
A	393	SER	-	expression tag	UNP Q14654
A	394	LEU	-	expression tag	UNP Q14654
A	395	GLU	-	expression tag	UNP Q14654
A	396	VAL	-	expression tag	UNP Q14654
A	397	LEU	-	expression tag	UNP Q14654
A	398	PHE	-	expression tag	UNP Q14654
A	399	GLN	-	expression tag	UNP Q14654
A	400	GLY	-	expression tag	UNP Q14654
D	-5	SER	-	expression tag	UNP Q14654
D	-4	ALA	-	expression tag	UNP Q14654
D	-3	SER	-	expression tag	UNP Q14654
D	-2	ALA	-	expression tag	UNP Q14654
D	-1	SER	-	expression tag	UNP Q14654
D	0	ALA	-	expression tag	UNP Q14654

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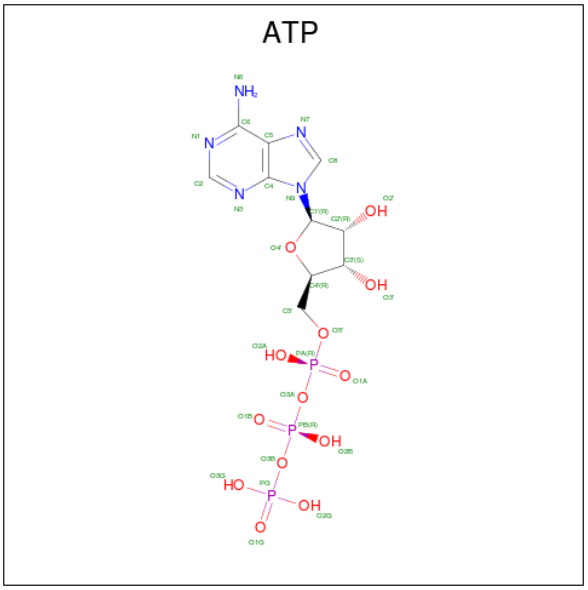
Chain	Residue	Modelled	Actual	Comment	Reference
D	391	SER	-	expression tag	UNP Q14654
D	392	ASN	-	expression tag	UNP Q14654
D	393	SER	-	expression tag	UNP Q14654
D	394	LEU	-	expression tag	UNP Q14654
D	395	GLU	-	expression tag	UNP Q14654
D	396	VAL	-	expression tag	UNP Q14654
D	397	LEU	-	expression tag	UNP Q14654
D	398	PHE	-	expression tag	UNP Q14654
D	399	GLN	-	expression tag	UNP Q14654
D	400	GLY	-	expression tag	UNP Q14654
B	-5	SER	-	expression tag	UNP Q14654
B	-4	ALA	-	expression tag	UNP Q14654
B	-3	SER	-	expression tag	UNP Q14654
B	-2	ALA	-	expression tag	UNP Q14654
B	-1	SER	-	expression tag	UNP Q14654
B	0	ALA	-	expression tag	UNP Q14654
B	391	SER	-	expression tag	UNP Q14654
B	392	ASN	-	expression tag	UNP Q14654
B	393	SER	-	expression tag	UNP Q14654
B	394	LEU	-	expression tag	UNP Q14654
B	395	GLU	-	expression tag	UNP Q14654
B	396	VAL	-	expression tag	UNP Q14654
B	397	LEU	-	expression tag	UNP Q14654
B	398	PHE	-	expression tag	UNP Q14654
B	399	GLN	-	expression tag	UNP Q14654
B	400	GLY	-	expression tag	UNP Q14654
C	-5	SER	-	expression tag	UNP Q14654
C	-4	ALA	-	expression tag	UNP Q14654
C	-3	SER	-	expression tag	UNP Q14654
C	-2	ALA	-	expression tag	UNP Q14654
C	-1	SER	-	expression tag	UNP Q14654
C	0	ALA	-	expression tag	UNP Q14654
C	391	SER	-	expression tag	UNP Q14654
C	392	ASN	-	expression tag	UNP Q14654
C	393	SER	-	expression tag	UNP Q14654
C	394	LEU	-	expression tag	UNP Q14654
C	395	GLU	-	expression tag	UNP Q14654
C	396	VAL	-	expression tag	UNP Q14654
C	397	LEU	-	expression tag	UNP Q14654
C	398	PHE	-	expression tag	UNP Q14654
C	399	GLN	-	expression tag	UNP Q14654
C	400	GLY	-	expression tag	UNP Q14654

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	E	1359	10077	6567	1699	1760	51	0	0
2	H	1359	10077	6567	1699	1760	51	0	0
2	G	1359	10077	6567	1699	1760	51	0	0
2	F	1359	10077	6567	1699	1760	51	0	0

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	A	1	62	20	10	26	6	0
3	A	1	62	20	10	26	6	0
3	D	1	31	10	5	13	3	0
3	C	1	31	10	5	13	3	0
3	E	1	31	10	5	13	3	0
3	H	1	31	10	5	13	3	0

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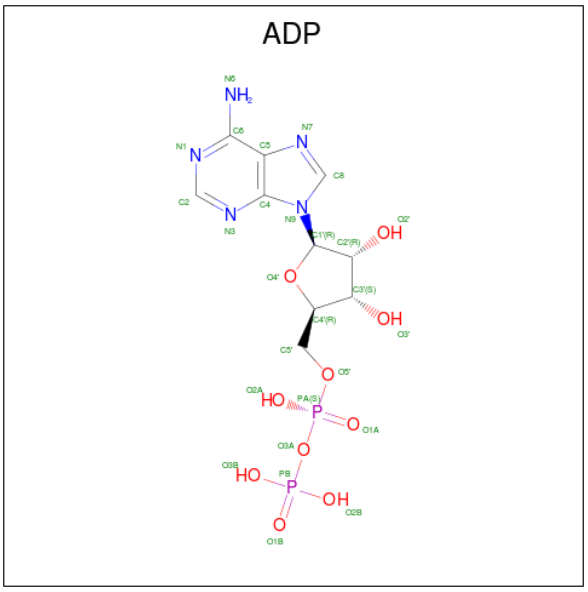
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
3	G	1	31	10	5	13	3	0
			Total	C	N	O	P	
3	F	1	31	10	5	13	3	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	E	1	27	10	5	10	2	0
			Total	C	N	O	P	
4	H	1	27	10	5	10	2	0
			Total	C	N	O	P	
4	G	1	27	10	5	10	2	0
			Total	C	N	O	P	
4	F	1	27	10	5	10	2	0

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	E	2	2	2	0
			Total	Mg	
5	H	2	2	2	0
			Total	Mg	
5	G	2	2	2	0

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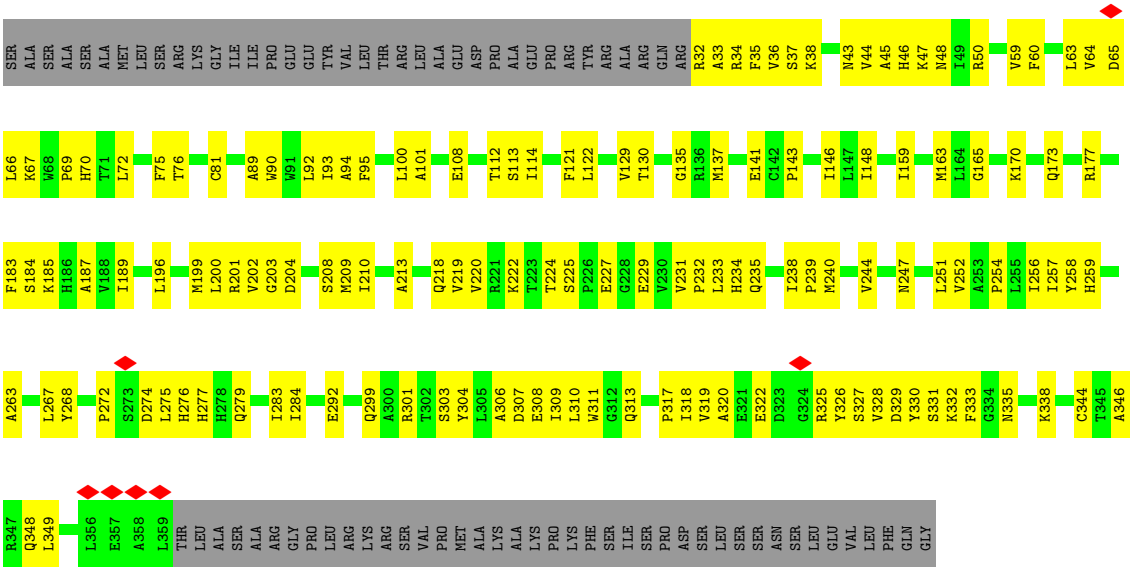
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	F	2	2	2	0

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.

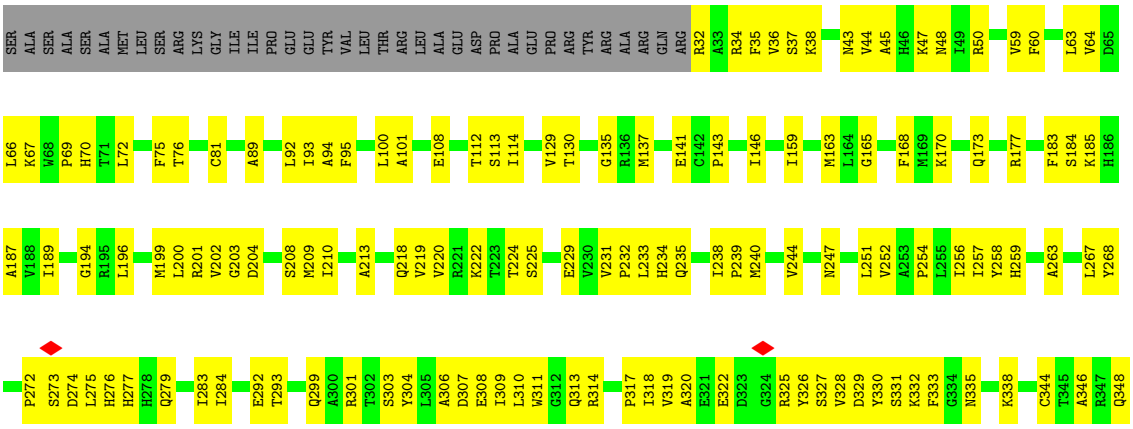
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

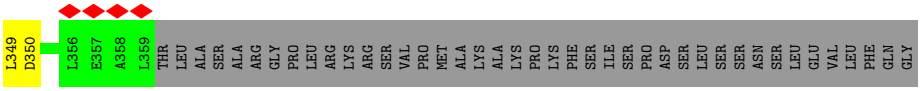
Chain A: 47% 34% 19%



• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

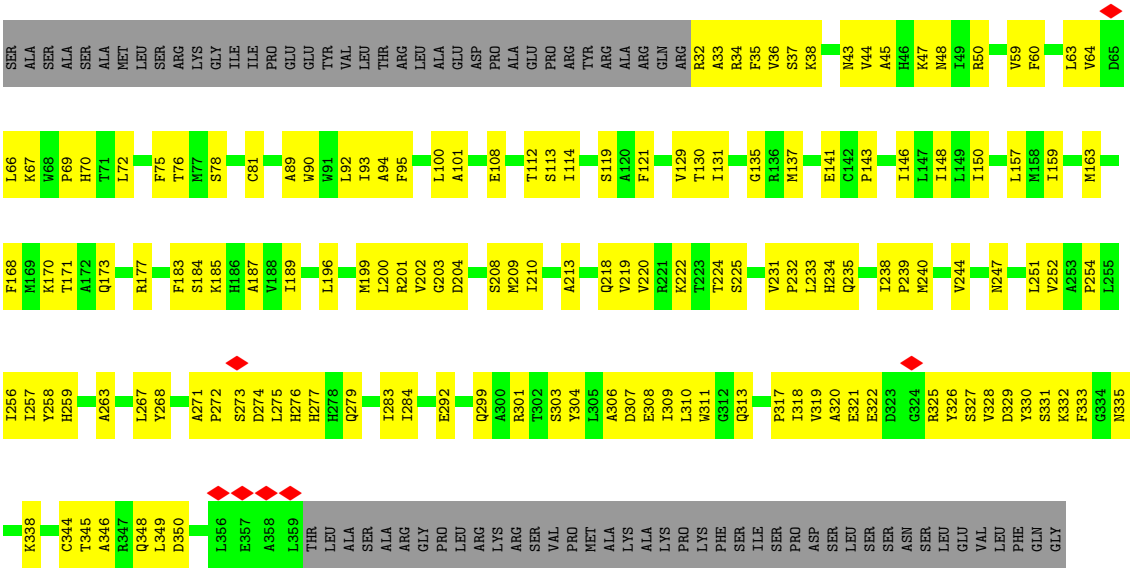
Chain D: 47% 34% 19%





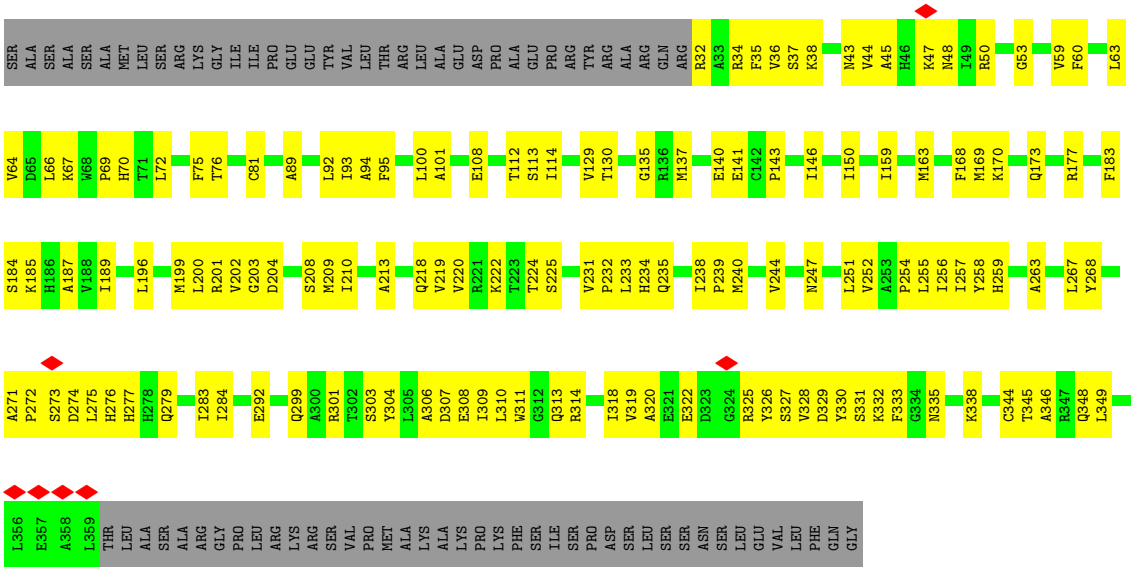
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain B:



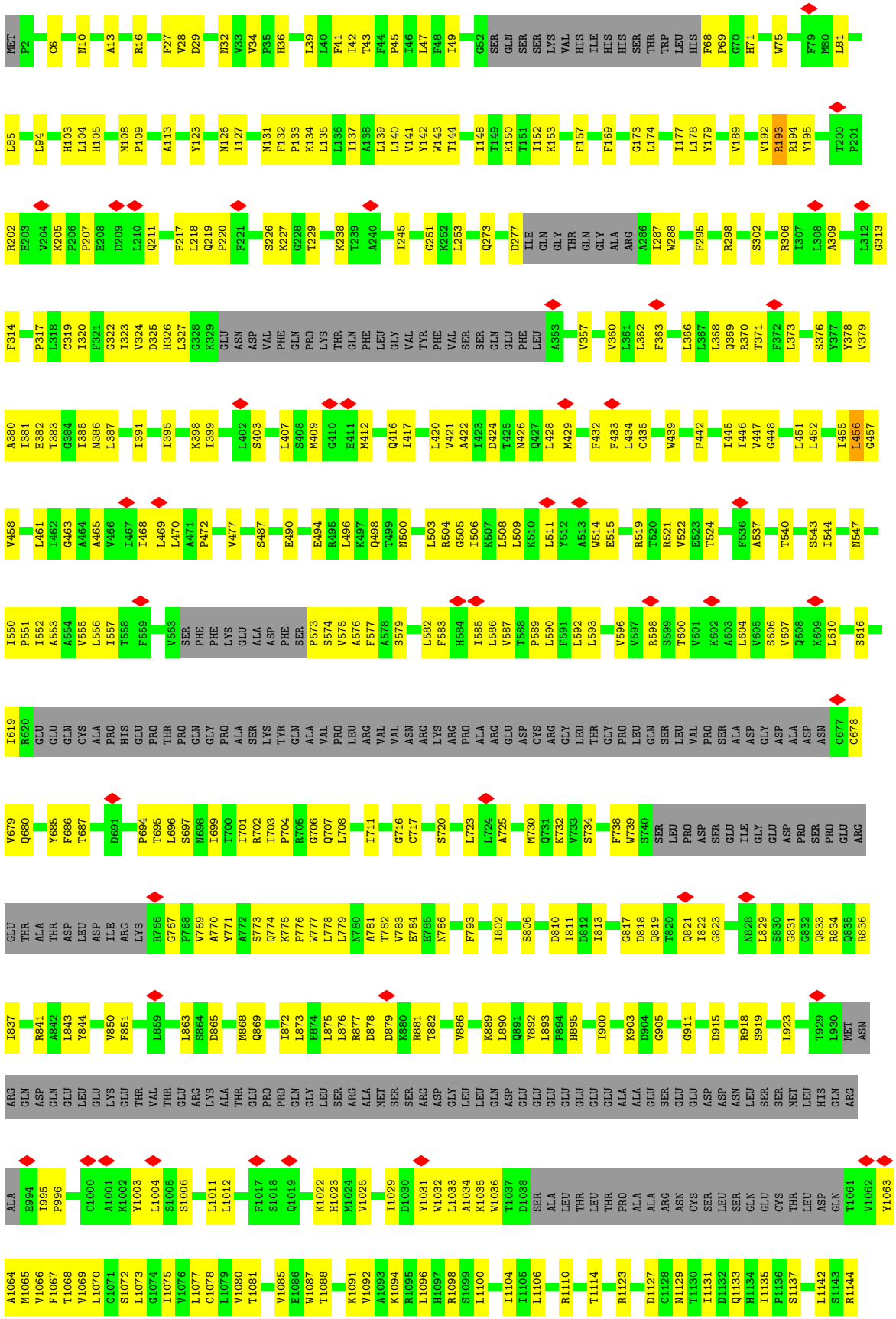
• Molecule 1: ATP-sensitive inward rectifier potassium channel 11

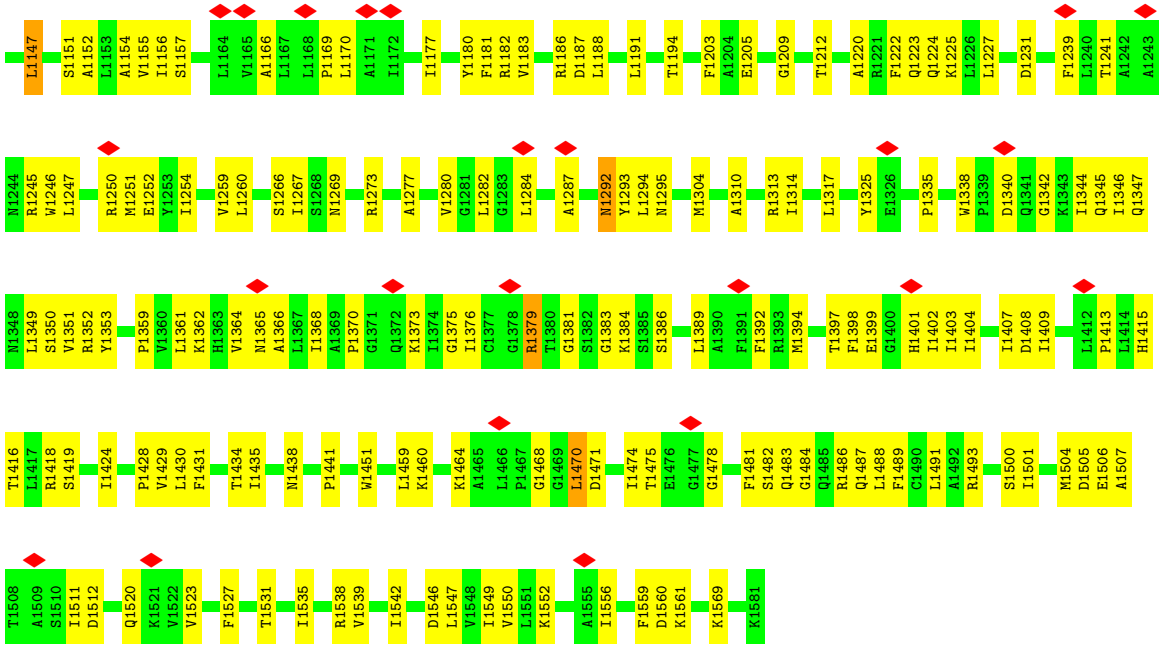
Chain C:



• Molecule 2: ATP-binding cassette sub-family C member 8

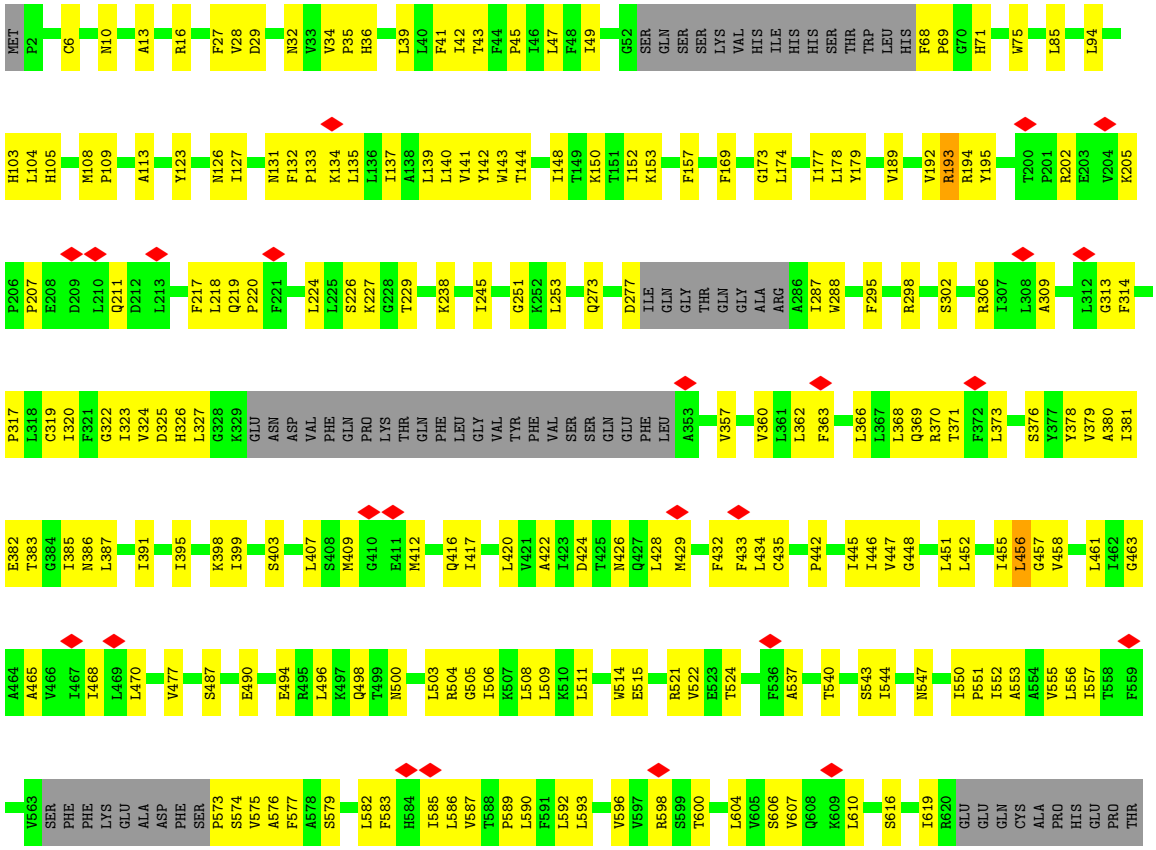
Chain E:

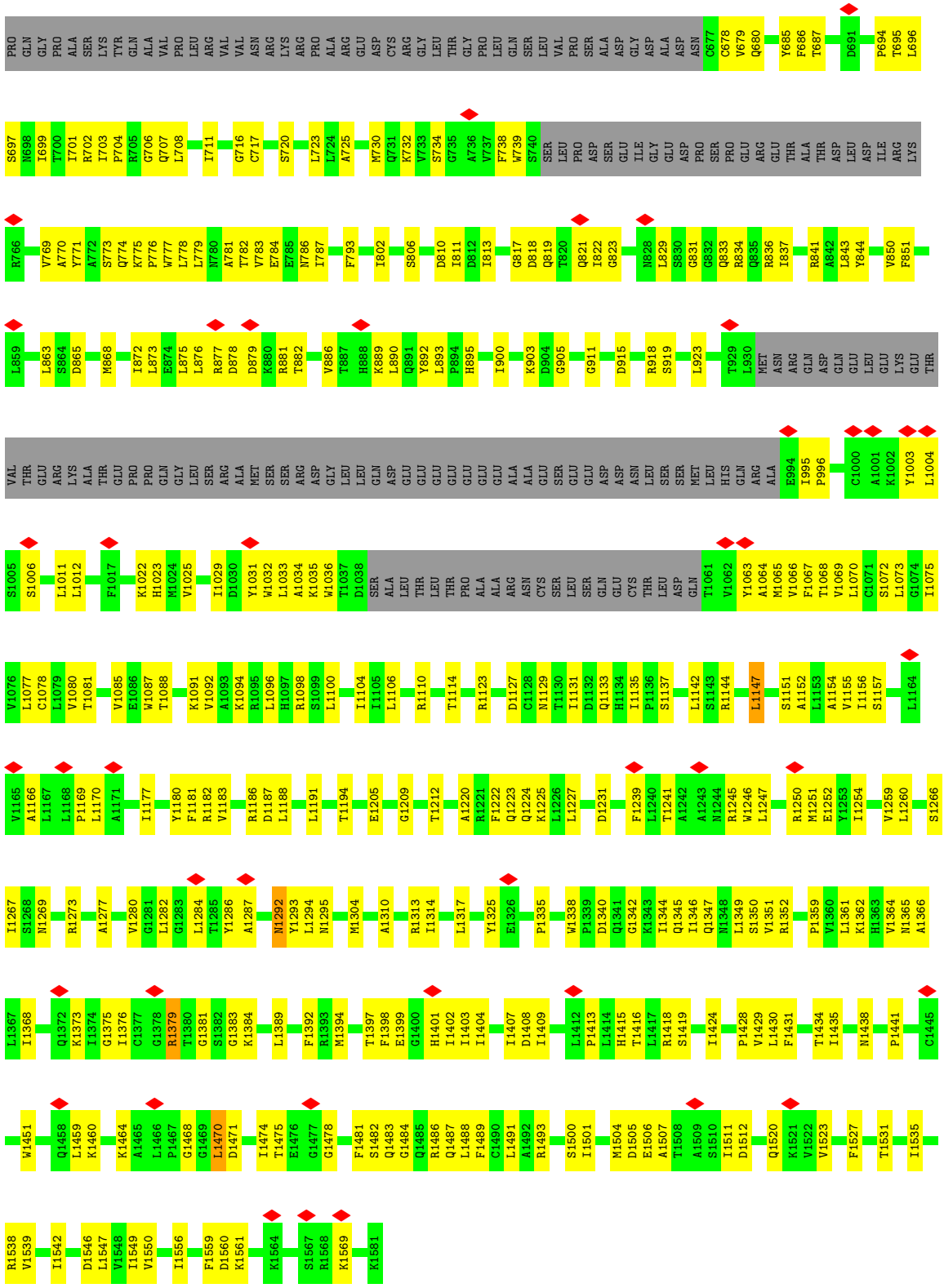

MET P2 C6 N10 A13 R16 F27 V28 D29 N32 V33 V34 P35 H36 L39 L40 F41 I42 T43 F44 P45 I46 L47 F48 I49 G52 SER GLN SER SER LYS VAL HIS ILE HIS HIS SER THR TRP LEU HIS F68 P69 G70 H71 W75 F79 M80 L81
L85 L94 H103 L104 H105 M108 P109 A113 Y123 N126 I127 N131 F132 P133 K134 L135 L136 I137 A138 L139 L140 Y141 Y142 W143 T144 I148 T149 K150 T151 I152 K153 F157 F169 G173 L174 I177 L178 Y179 V189 V192 R193 R194 Y195 T200 P201
R202 E203 V204 K205 P206 P207 E208 D209 L210 Q211 F217 L218 Q219 P220 F221 S226 K227 G228 T229 K238 T239 A240 I245 G251 K252 L253 Q273 D277 ILE GLN GLY THR GLN GLY ALA ARG A286 I287 W288 F295 R298 S302 R306 I307 L308 A309 L312 G313
F314 P317 L318 C319 I320 F321 G322 I323 V324 D325 H326 L327 G328 K329 GLU ASN ASP VAL PHE GLN PRO LYS THR GLN PHE LEU GLY VAL TYR PHE VAL SER SER GLN GLU PHE LEU A353 V357 V360 L361 L362 F363 L366 L367 L368 Q369 R370 T371 F372 L373 S376 Y377 Y378 V379
A380 I381 E382 T383 G384 I385 N386 L387 I391 I395 K398 I399 L402 S403 L407 S408 M409 G410 E411 M412 Q416 I417 L420 V421 A422 I423 D424 T425 N426 Q427 L428 M429 F432 F433 L434 C435 W439 P442 I445 I446 V447 G448 L451 L452 I455 L456 G457
V458 L461 I462 G463 A464 A465 V466 I467 I468 L469 L470 A471 P472 V477 S487 E490 E494 R495 L496 K497 Q498 T499 N500 L503 R504 G505 I506 K507 L508 L509 K510 L511 Y512 A513 W514 E515 R519 T520 R521 V522 E523 T524 F536 A537 T540 S543 I544 N547
I550 P551 I552 A553 A554 V555 L556 I557 T558 F559 V563 SER PHE PHE LYS GLU ALA ASP PHE SER P573 S574 V575 A576 F577 A578 S579 L582 F583 H584 I585 L586 V587 T588 P589 L590 F591 L592 L593 V596 V597 R598 S599 T600 V601 K602 A603 L604 V605 S606 V607 Q608 K609 L610 S616
I619 R620 GLU GLU GLN CYS ALA PRO HIS GLU PRO THR PRO GLN GLY PRO ALA SER LYS TYR GLN ALA VAL PRO LEU ARG VAL VAL ASN ARG LYS ARG PRO ALA ARG GLU ASP CYS ARG GLY LEU THR GLY PRO LEU GLN SER LEU VAL PRO SER ALA ASP GLY ASP ALA ASP ASN C677 C678
V679 Q680 Y685 F686 T687 D691 P694 T695 L696 S697 N698 I699 T700 I701 R702 I703 P704 R705 G706 Q707 L708 I711 G716 C717 S720 L723 L724 A725 M730 Q731 K732 V733 S734 F738 W739 S740 SER LEU PRO ASP SER GLU ILE GLY GLU ASP PRO SER PRO GLU ARG
GLU THR ALA THR ASP LEU ASP ILE ARG LYS R766 G767 P768 V769 A770 Y771 A772 S773 Q774 K775 P776 W777 L778 L779 N780 A781 T782 V783 E784 E785 N786 F793 I802 S806 D810 I811 D812 I813 G817 D818 Q819 T820 Q821 I822 G823 N828 L829 S830 G831 G832 Q833 R834 Q835 R836
I837 R841 A842 L843 Y844 V850 F851 L859 L863 S864 D865 M868 Q869 I872 L873 E874 L875 L876 R877 D878 D879 K880 R881 T882 V886 K889 L890 Q891 Y892 L893 P894 H895 I900 K903 D904 G905 G911 D915 R918 S919 L923 T929 L930 MET ASN
ARG GLN ASP GLN GLU LEU GLU LYS GLU THR VAL THR GLU ARG LYS ALA THR GLU PRO PRO GLN GLY LEU SER ARG ALA MET SER SER ARG ASP GLY LEU LEU GLN ASP GLU GLU GLU GLU GLU GLU GLU ALA ALA GLU SER GLU GLU ASP ASN LEU SER SER MET LEU HIS GLN ARG
ALA E994 I995 P996 C1000 A1001 K1002 Y1003 L1004 S1005 S1006 L1011 L1012 F1017 S1018 Q1019 K1022 H1023 M1024 V1025 I1029 D1030 Y1031 W1032 L1033 A1034 K1035 W1036 T1037 D1038 SER ALA LEU THR LEU THR PRO ALA ALA ARG ASN CYS SER LEU SER LYS THR LEU ASP GLN T1061 V1062 Y1063
A1064 M1065 V1066 F1067 T1068 V1069 L1070 C1071 S1072 L1073 G1074 I1075 V1076 L1077 C1078 L1079 V1080 T1081 V1085 E1086 W1087 T1088 K1091 V1092 A1093 K1094 R1095 L1096 H1097 R1098 S1099 L1100 I1104 I1105 L1106 R1110 T1114 R1123 D1127 C1128 N1129 T1130 I1131 D1132 Q1133 H1134 I1135 P1136 S1137 L1142 S1143 R1144



- Molecule 2: ATP-binding cassette sub-family C member 8

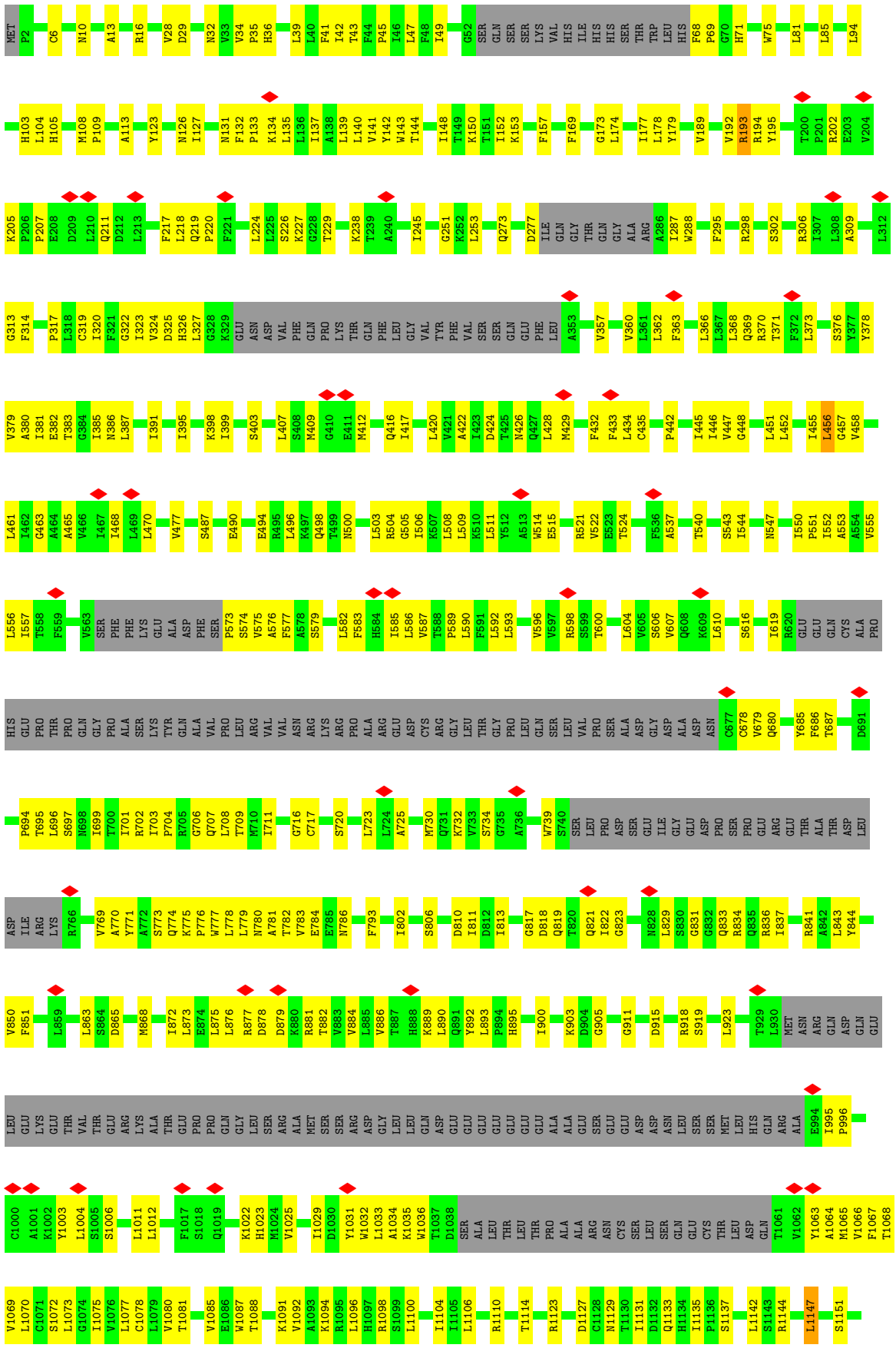
Chain H:

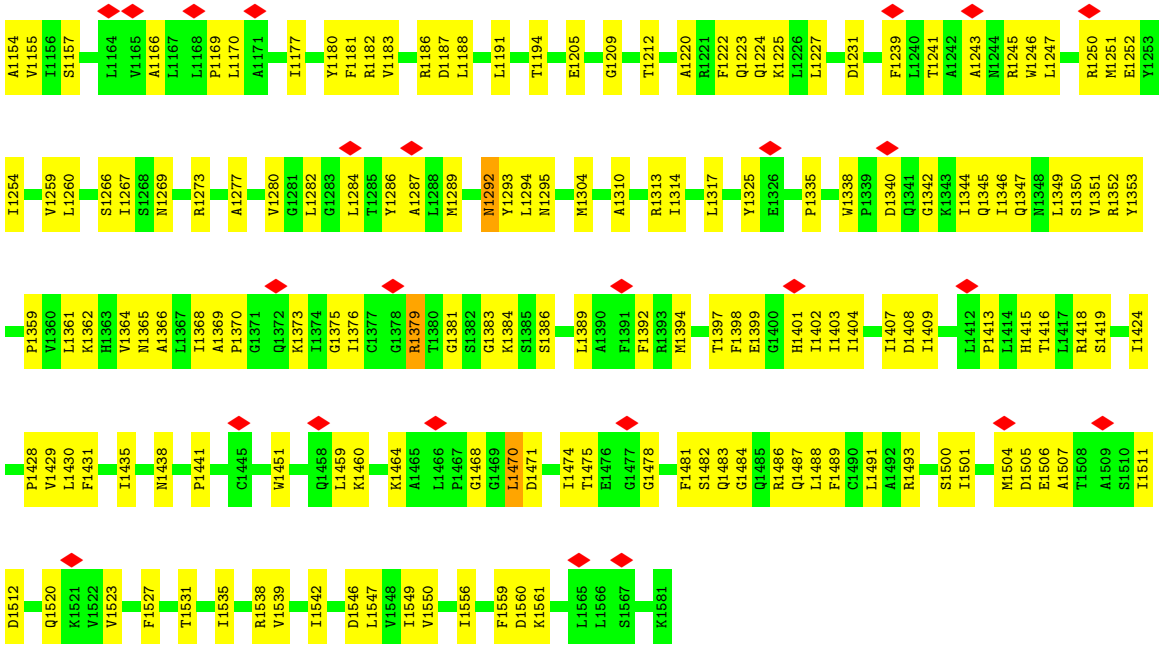




- Molecule 2: ATP-binding cassette sub-family C member 8

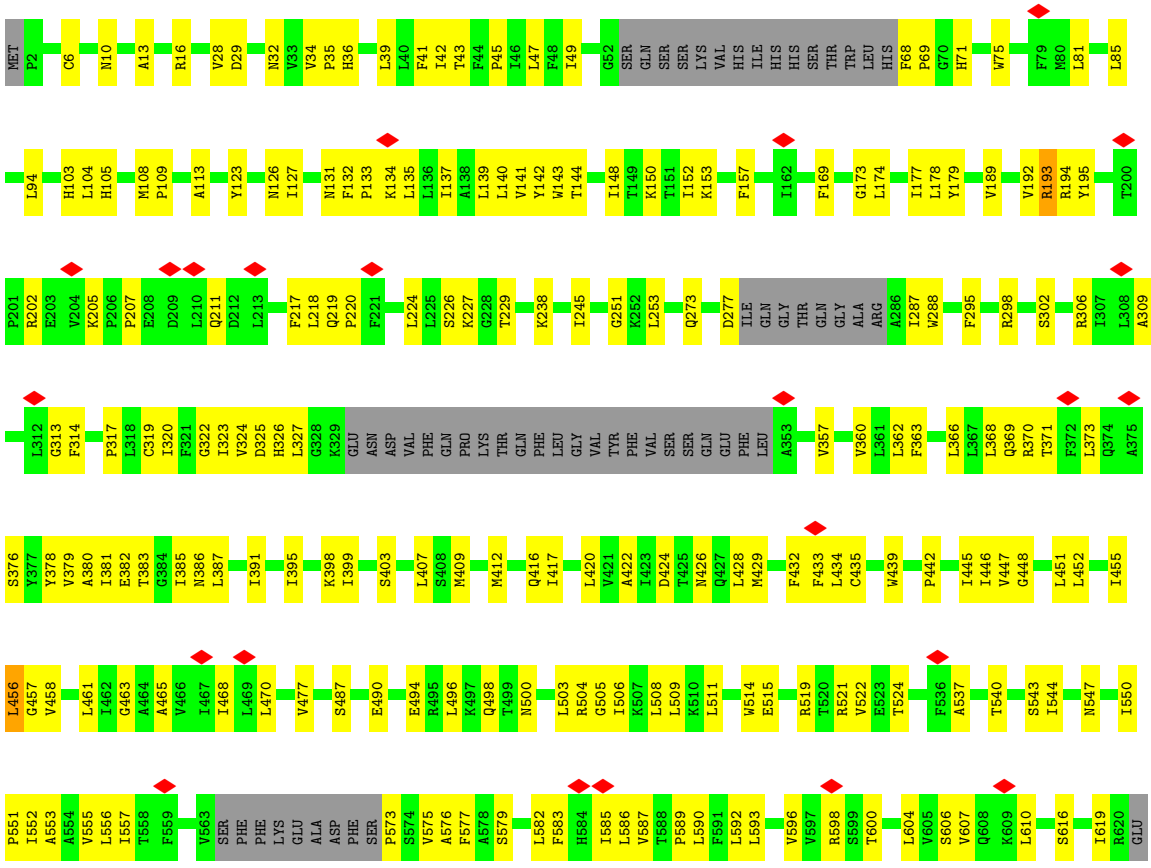
Chain G:

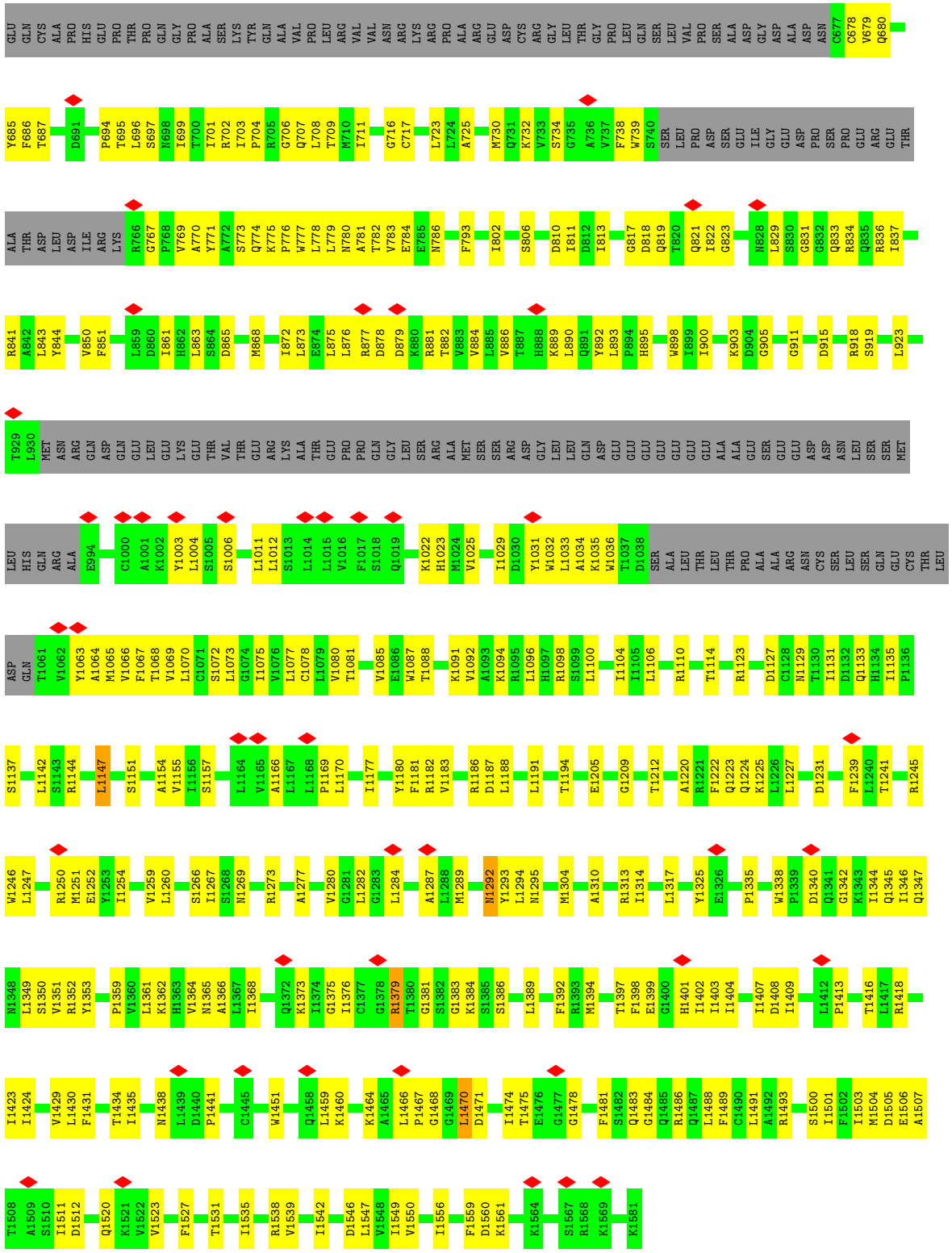

MET P2 C6 N10 A13 R16 V28 D29 N32 V33 V34 P35 H36 L39 L40 F41 I42 T43 F44 P45 I46 L47 F48 I49 G52 SER GLN SER SER LYS VAL HIS ILE HIS HIS SER THR TRP LEU HIS F68 P69 G70 H71 W75 L81 L85 L94
H103 L104 H105 M108 P109 A113 Y123 N126 I127 N131 F132 P133 K134 L135 L136 I137 A138 L139 L140 V141 Y142 W143 T144 I148 T149 K150 T151 I152 K153 F157 F169 G173 L174 I177 L178 Y179 V189 V192 R193 R194 Y195 T200 P201 R202 E203 V204
K205 P206 P207 E208 D209 L210 Q211 D212 L213 F217 L218 Q219 P220 F221 L224 L225 S226 K227 G228 T229 K238 T239 A240 I245 G251 K252 L253 Q273 D277 ILE GLN GLY THR GLN GLY ALA ARG A286 I287 W288 F295 R298 S302 R306 I307 I308 A309 L312
G313 F314 P317 L318 C319 I320 F321 G322 I323 V324 D325 H326 L327 G328 K329 GLU ASN ASP VAL PHE GLN PRO LYS THR GLN PHE LEU GLY VAL TYR PHE VAL SER SER GLN GLU PHE LEU A353 V357 V360 L361 L362 F363 L366 L367 L368 Q369 R370 T371 F372 L373 S376 Y377 Y378
V379 A380 I381 E382 T383 G384 I385 N386 L387 I391 I395 K398 I399 S403 L407 S408 M409 G410 E411 M412 Q416 I417 L420 V421 A422 I423 D424 T425 N426 Q427 L428 M429 F432 F433 L434 C435 P442 I445 I446 V447 G448 L451 L452 I455 L456 G457 V458
L461 I462 G463 A464 A465 V466 I467 I468 L469 L470 V477 S487 E490 E494 R495 L496 K497 Q498 T499 N500 L503 R504 G505 I506 K507 L508 L509 K510 L511 Y512 A513 W514 E515 R521 V522 E523 T524 F536 A537 T540 S543 I544 N547 I550 P551 I552 A553 A554 V555
L556 I557 T558 F559 V563 SER PHE PHE LYS GLU ALA ASP PHE SER P573 S574 V575 A576 F577 A578 S579 L582 F583 H584 I585 L586 V587 T588 P589 L590 F591 L592 L593 V596 V597 R598 S599 T600 L604 V605 S606 V607 Q608 K609 L610 S616 I619 R620 GLU GLU GLN CYS ALA PRO
HIS GLU PRO THR PRO GLN GLY PRO ALA SER LYS TYR GLN ALA VAL PRO LEU ARG VAL VAL ASN ARG LYS ARG PRO ALA ARG GLU ASP CYS ARG GLY LEU THR GLY PRO LEU GLN SER LEU VAL PRO SER ALA ASP GLY ASP ALA ASP ASN G677 C678 V679 Q680 Y685 F686 T687 D691
P694 T695 L696 S697 N698 I699 T700 I701 R702 I703 P704 R705 G706 Q707 L708 T709 M710 I711 G716 C717 S720 L723 L724 A725 M730 Q731 K732 V733 S734 G735 A736 W739 S740 SER LEU PRO ASP SER GLU ILE GLY GLU ASP PRO SER PRO GLU ARG GLU THR ALA THR ASP LEU
ASP ILE ARG LYS R766 V769 A770 Y771 A772 S773 Q774 K775 P776 W777 L778 L779 N780 A781 T782 V783 E784 E785 N786 F793 I802 S806 D810 I811 D812 I813 G817 D818 Q819 T820 Q821 I822 G823 N828 L829 S830 G831 G832 Q833 R834 Q835 R836 I837 R841 A842 L843 Y844
V850 F851 L859 L863 S864 D865 M868 I872 L873 E874 L875 L876 R877 D878 D879 K880 R881 T882 V883 V884 L885 V886 T887 H888 K889 L890 Q891 Y892 L893 P894 H895 I900 K903 D904 G905 G911 D915 R918 S919 L923 T929 L930 MET ASN ARG GLN ASP GLN GLU
LEU GLU LYS GLU THR VAL THR GLU ARG LYS ALA THR GLU PRO PRO GLN GLY LEU SER ARG ALA MET SER SER ARG ASP GLY LEU LEU GLN ASP GLU GLU GLU GLU GLU GLU GLU GLU ALA ALA ALA GLU SER GLU GLU ASP ASP ASN LEU SER SER MET LEU HIS GLN ARG ALA E994 I995 P996
C1000 A1001 K1002 Y1003 L1004 S1005 S1006 L1011 L1012 F1017 S1018 Q1019 K1022 H1023 M1024 V1025 I1029 D1030 Y1031 W1032 L1033 A1034 K1035 W1036 T1037 D1038 SER ALA ALA LEU THR LEU THR PRO ALA ALA ALA ARG ASN CYS SER LEU SER GLN GLU CYS THR LEU ASP GLN T1061 V1062 Y1063 A1064 M1065 V1066 F1067 T1068
V1069 L1070 C1071 S1072 L1073 G1074 I1075 V1076 L1077 C1078 L1079 V1080 T1081 V1085 E1086 W1087 T1088 K1091 V1092 A1093 K1094 R1095 L1096 H1097 R1098 S1099 L1100 I1104 I1105 L1106 R1110 T1114 R1123 D1127 C1128 N1129 T1130 I1131 D1132 Q1133 H1134 I1135 P1136 S1137 L1142 S1143 R1144 L1147 S1151



- Molecule 2: ATP-binding cassette sub-family C member 8

Chain F:




GLU GLN CYS ALA PRO HIS GLU PRO THR PRO GLN GLY PRO ALA SER LYS TYR GLN ALA VAL PRO LEU ARG VAL VAL ASN ARG LYS ARG PRO ALA ARG GLU ASP CYS ARG GLY LEU THR GLY PRO LEU GLN SER LEU VAL PRO SER ALA ASP GLY ASP ALA ASP ASN C677 C678 V679 Q680
Y685 F686 T687 D691 P694 T695 L696 S697 N698 I699 T700 I701 R702 I703 P704 R705 G706 Q707 L708 T709 M710 I711 G716 C717 L723 L724 A725 M730 Q731 K732 V733 S734 G735 A736 V737 F738 W739 S740 SER LEU PRO ASP SER GLU ILE GLY GLU ASP PRO SER PRO GLU ARG GLU THR
ALA THR ASP LEU ASP ILE ARG LYS R766 G767 P768 V769 A770 Y771 A772 S773 Q774 K775 P776 W777 L778 L779 N780 A781 T782 V783 E784 E785 N786 F793 I802 S806 D810 I811 D812 I813 G817 D818 Q819 T820 Q821 I822 G823 N828 L829 S830 G831 G832 Q833 R834 Q835 R836 I837
R841 A842 L843 Y844 V850 F851 L859 D860 I861 H862 L863 S864 D865 M868 I872 L873 E874 L875 L876 R877 D878 D879 K880 R881 T882 V883 V884 L885 V886 T887 H888 K889 L890 Q891 Y892 L893 P894 H895 W898 I899 I900 K903 D904 G905 G911 D915 R918 S919 L923
T929 L930 MET ASN ARG GLN ASP GLN GLU LEU GLU LYS GLU THR VAL THR GLU ARG LYS ALA THR GLU PRO PRO GLN GLY LEU SER ARG ALA MET SER SER ARG ASP GLY LEU LEU GLN ASP GLU GLU GLU GLU GLU GLU GLU ALA ALA GLU SER GLU GLU ASP ASP ASN LEU SER SER MET
LEU HIS GLN ARG ALA E994 C1000 A1001 K1002 Y1003 L1004 S1005 S1006 L1011 L1012 S1013 L1014 L1015 V1016 F1017 S1018 Q1019 K1022 H1023 M1024 V1025 I1029 D1030 Y1031 W1032 L1033 A1034 K1035 W1036 T1037 D1038 SER ALA LEU THR LEU THR PRO ALA ALA ARG ASN CYS CYS SER LEU SER GLN GLU CYS THR LEU
ASP GLN T1061 V1062 Y1063 A1064 M1065 V1066 F1067 T1068 V1069 L1070 C1071 S1072 L1073 G1074 I1075 V1076 L1077 C1078 L1079 V1080 T1081 V1085 E1086 W1087 T1088 K1091 V1092 A1093 K1094 R1095 L1096 H1097 R1098 S1099 L1100 I1104 I1105 L1106 R1110 T1114 R1123 D1127 C1128 N1129 T1130 I1131 D1132 Q1133 H1134 I1135 P1136
S1137 L1142 S1143 R1144 L1147 S1151 A1154 V1155 I1156 S1157 L1164 V1165 A1166 L1167 L1168 P1169 L1170 I1177 Y1180 F1181 R1182 V1183 R1186 D1187 L1188 L1191 T1194 E1205 G1209 T1212 A1220 R1221 F1222 Q1223 Q1224 K1225 L1226 L1227 D1231 F1239 L1240 T1241 R1245
W1246 L1247 R1250 M1251 E1252 Y1253 I1254 V1259 L1260 S1266 I1267 S1268 N1269 R1273 A1277 V1280 G1281 L1282 G1283 L1284 A1287 L1288 M1289 N1292 Y1293 L1294 N1295 M1304 A1310 R1313 I1314 L1317 Y1325 E1326 P1335 W1338 P1339 D1340 Q1341 G1342 K1343 I1344 Q1345 I1346 Q1347
N1348 L1349 S1350 V1351 R1352 Y1353 P1359 V1360 L1361 K1362 H1363 V1364 N1365 A1366 L1367 I1368 Q1372 K1373 I1374 G1375 I1376 C1377 G1378 R1379 T1380 G1381 S1382 G1383 K1384 S1385 S1386 L1389 F1392 R1393 M1394 T1397 F1398 E1399 G1400 H1401 I1402 I1403 I1404 I1407 D1408 I1409 L1412 P1413 T1416 L1417 R1418
I1423 I1424 V1429 L1430 F1431 T1434 I1435 N1438 L1439 D1440 P1441 C1445 W1451 Q1458 L1459 K1460 K1464 A1465 L1466 P1467 G1468 G1469 L1470 D1471 I1474 T1475 E1476 G1477 G1478 F1481 S1482 Q1483 G1484 Q1485 R1486 Q1487 L1488 F1489 C1490 L1491 A1492 R1493 S1500 I1501 F1502 I1503 M1504 D1505 E1506 A1507
T1508 A1509 S1510 I1511 D1512 Q1520 K1521 V1522 V1523 F1527 T1531 I1535 R1538 V1539 I1542 D1546 L1547 Y1548 I1549 V1550 I1556 F1559 D1560 K1561 K1564 S1567 R1568 K1569 K1581

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47282	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 ($e^-/Å^2$)	1.18	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	1.014	Depositor
Minimum map value	-0.760	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.0343	Depositor
Map size (Å)	390.0, 390.0, 390.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3, 1.3, 1.3	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.36	0/2563	0.51	0/3490
1	B	0.36	0/2563	0.51	0/3490
1	C	0.36	0/2563	0.51	0/3490
1	D	0.36	0/2563	0.51	0/3490
2	E	0.32	0/10282	0.50	2/14031 (0.0%)
2	F	0.32	0/10282	0.50	2/14031 (0.0%)
2	G	0.32	0/10282	0.50	2/14031 (0.0%)
2	H	0.32	0/10282	0.50	2/14031 (0.0%)
All	All	0.33	0/51380	0.50	8/70084 (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
2	E	0	2
2	F	0	2
2	G	0	2
2	H	0	2
All	All	0	8

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})
2	H	1294	LEU	CA-CB-CG	5.39	127.69	115.30
2	G	1294	LEU	CA-CB-CG	5.37	127.64	115.30
2	F	1294	LEU	CA-CB-CG	5.37	127.64	115.30
2	E	1294	LEU	CA-CB-CG	5.35	127.61	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1470	LEU	CA-CB-CG	5.18	127.21	115.30

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	193	ARG	Peptide
2	E	202	ARG	Peptide
2	G	193	ARG	Peptide
2	H	193	ARG	Peptide
2	H	202	ARG	Peptide

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2506	0	2494	129	0
1	B	2506	0	2494	130	0
1	C	2506	0	2494	120	0
1	D	2506	0	2494	122	0
2	E	10077	0	9922	408	0
2	F	10077	0	9922	407	0
2	G	10077	0	9922	406	0
2	H	10077	0	9922	404	0
3	A	62	0	24	8	0
3	C	31	0	12	3	0
3	D	31	0	12	4	0
3	E	31	0	12	5	0
3	F	31	0	12	2	0
3	G	31	0	12	4	0
3	H	31	0	12	5	0
4	E	27	0	12	2	0
4	F	27	0	12	2	0
4	G	27	0	12	2	0
4	H	27	0	12	2	0
5	E	2	0	0	0	0
5	F	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	G	2	0	0	0	0
5	H	2	0	0	0	0
All	All	50696	0	49808	2070	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 21.

The worst 5 of 2070 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)
2:H:1501:ILE:HG22	2:H:1531:THR:HB	1.55	0.88
2:G:1501:ILE:HG22	2:G:1531:THR:HB	1.55	0.88
2:F:1501:ILE:HG22	2:F:1531:THR:HB	1.55	0.87
2:H:1459:LEU:HD21	2:H:1488:LEU:HB3	1.58	0.86
2:E:1501:ILE:HG22	2:E:1531:THR:HB	1.55	0.85

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	326/406 (80%)	293 (90%)	32 (10%)	1 (0%)	41	76
1	B	326/406 (80%)	293 (90%)	32 (10%)	1 (0%)	41	76
1	C	326/406 (80%)	293 (90%)	32 (10%)	1 (0%)	41	76
1	D	326/406 (80%)	292 (90%)	33 (10%)	1 (0%)	41	76
2	E	1341/1581 (85%)	1242 (93%)	97 (7%)	2 (0%)	51	85
2	F	1341/1581 (85%)	1241 (92%)	98 (7%)	2 (0%)	51	85
2	G	1341/1581 (85%)	1240 (92%)	99 (7%)	2 (0%)	51	85
2	H	1341/1581 (85%)	1241 (92%)	98 (7%)	2 (0%)	51	85

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6668/7948 (84%)	6135 (92%)	521 (8%)	12 (0%)	50 81

5 of 12 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	E	194	ARG
2	H	194	ARG
2	G	194	ARG
2	F	194	ARG
1	A	48	ASN

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	265/348 (76%)	265 (100%)	0	100 100
1	B	265/348 (76%)	265 (100%)	0	100 100
1	C	265/348 (76%)	265 (100%)	0	100 100
1	D	265/348 (76%)	265 (100%)	0	100 100
2	E	1004/1368 (73%)	998 (99%)	6 (1%)	86 91
2	F	1004/1368 (73%)	998 (99%)	6 (1%)	86 91
2	G	1004/1368 (73%)	998 (99%)	6 (1%)	86 91
2	H	1004/1368 (73%)	998 (99%)	6 (1%)	86 91
All	All	5076/6864 (74%)	5052 (100%)	24 (0%)	89 93

5 of 24 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	G	1147	LEU
2	G	1379	ARG
2	G	1295	ASN
2	F	547	ASN
2	H	547	ASN

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

Mol	Chain	Res	Type
2	G	103	HIS
2	F	36	HIS
2	G	188	ASN
2	G	1102	ASN
2	F	416	GLN

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 20 ligands modelled in this entry, 8 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	ATP	A	502	-	26,33,33	0.91	1 (3%)	31,52,52	1.76	6 (19%)
3	ATP	C	501	-	26,33,33	0.93	1 (3%)	31,52,52	1.74	5 (16%)
4	ADP	F	2001	5	24,29,29	0.92	1 (4%)	29,45,45	1.49	4 (13%)
3	ATP	A	501	-	26,33,33	0.92	1 (3%)	31,52,52	1.73	5 (16%)
3	ATP	D	501	-	26,33,33	0.91	1 (3%)	31,52,52	1.74	5 (16%)
4	ADP	G	2001	5	24,29,29	0.92	1 (4%)	29,45,45	1.48	4 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	ATP	H	2004	5	26,33,33	0.93	1 (3%)	31,52,52	1.67	6 (19%)
3	ATP	G	2004	5	26,33,33	0.92	1 (3%)	31,52,52	1.67	6 (19%)
4	ADP	H	2001	5	24,29,29	0.92	1 (4%)	29,45,45	1.48	4 (13%)
3	ATP	F	2004	5	26,33,33	0.94	1 (3%)	31,52,52	1.67	6 (19%)
4	ADP	E	2001	5	24,29,29	0.92	1 (4%)	29,45,45	1.48	4 (13%)
3	ATP	E	2004	5	26,33,33	0.92	1 (3%)	31,52,52	1.67	6 (19%)

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	ATP	A	502	-	-	4/18/38/38	0/3/3/3
3	ATP	C	501	-	-	4/18/38/38	0/3/3/3
4	ADP	F	2001	5	-	3/12/32/32	0/3/3/3
3	ATP	A	501	-	-	4/18/38/38	0/3/3/3
3	ATP	D	501	-	-	5/18/38/38	0/3/3/3
4	ADP	G	2001	5	-	3/12/32/32	0/3/3/3
3	ATP	H	2004	5	-	3/18/38/38	0/3/3/3
3	ATP	G	2004	5	-	3/18/38/38	0/3/3/3
4	ADP	H	2001	5	-	3/12/32/32	0/3/3/3
3	ATP	F	2004	5	-	3/18/38/38	0/3/3/3
4	ADP	E	2001	5	-	3/12/32/32	0/3/3/3
3	ATP	E	2004	5	-	3/18/38/38	0/3/3/3

The worst 5 of 12 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	2001	ADP	C5-C4	2.43	1.47	1.40
3	C	501	ATP	C5-C4	2.40	1.47	1.40
4	H	2001	ADP	C5-C4	2.39	1.47	1.40
3	A	501	ATP	C5-C4	2.38	1.47	1.40
3	A	502	ATP	C5-C4	2.38	1.47	1.40

The worst 5 of 61 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	502	ATP	PA-O3A-PB	-4.68	116.77	132.83
3	D	501	ATP	PA-O3A-PB	-4.66	116.85	132.83
3	C	501	ATP	PA-O3A-PB	-4.59	117.08	132.83
3	A	501	ATP	PA-O3A-PB	-4.57	117.14	132.83
3	D	501	ATP	PB-O3B-PG	-4.23	118.31	132.83

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	ATP	C5'-O5'-PA-O1A
3	A	501	ATP	C5'-O5'-PA-O3A
3	A	502	ATP	C5'-O5'-PA-O3A
3	D	501	ATP	C5'-O5'-PA-O1A
3	C	501	ATP	C5'-O5'-PA-O1A

There are no ring outliers.

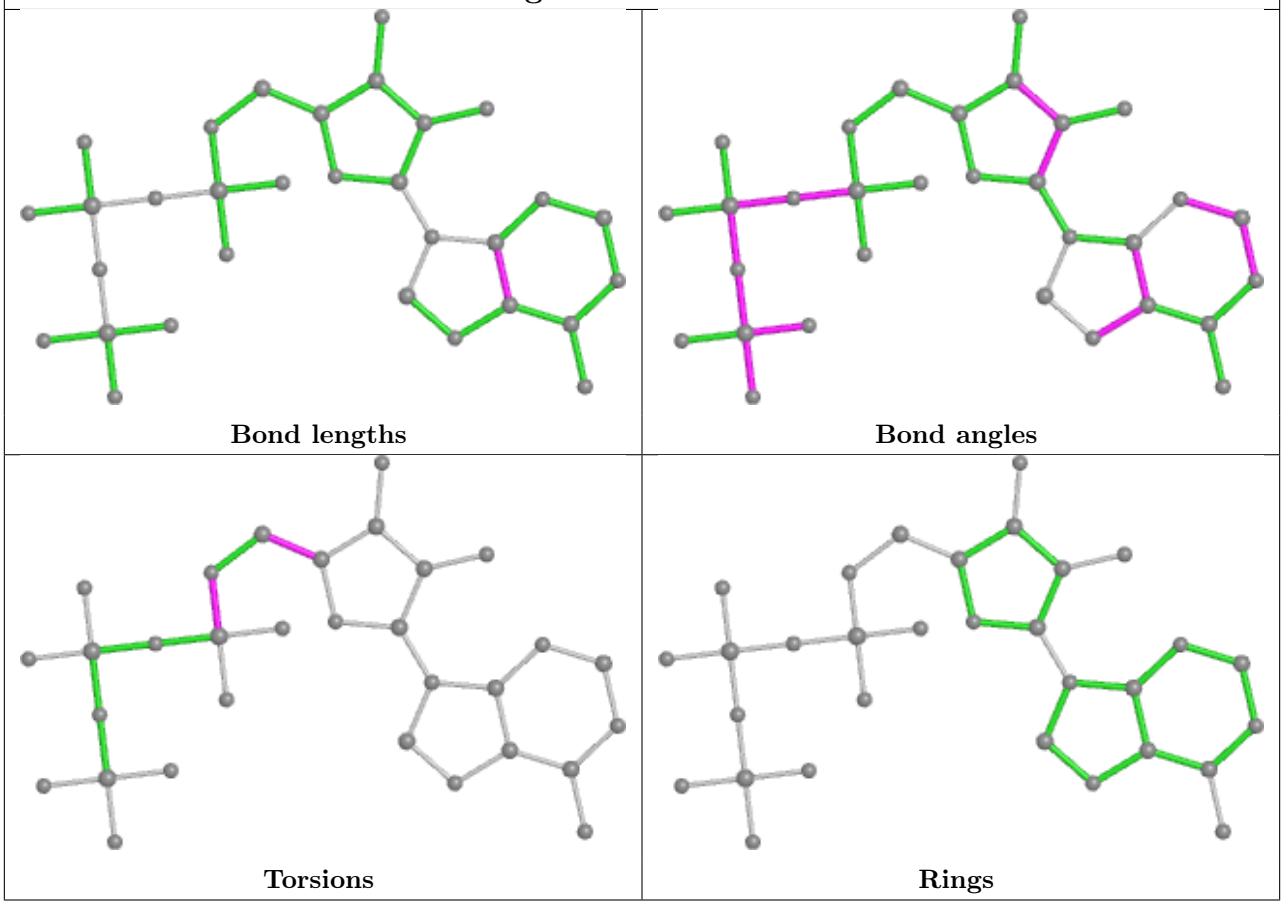
12 monomers are involved in 39 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	502	ATP	5	0
3	C	501	ATP	3	0
4	F	2001	ADP	2	0
3	A	501	ATP	3	0
3	D	501	ATP	4	0
4	G	2001	ADP	2	0
3	H	2004	ATP	5	0
3	G	2004	ATP	4	0
4	H	2001	ADP	2	0
3	F	2004	ATP	2	0
4	E	2001	ADP	2	0
3	E	2004	ATP	5	0

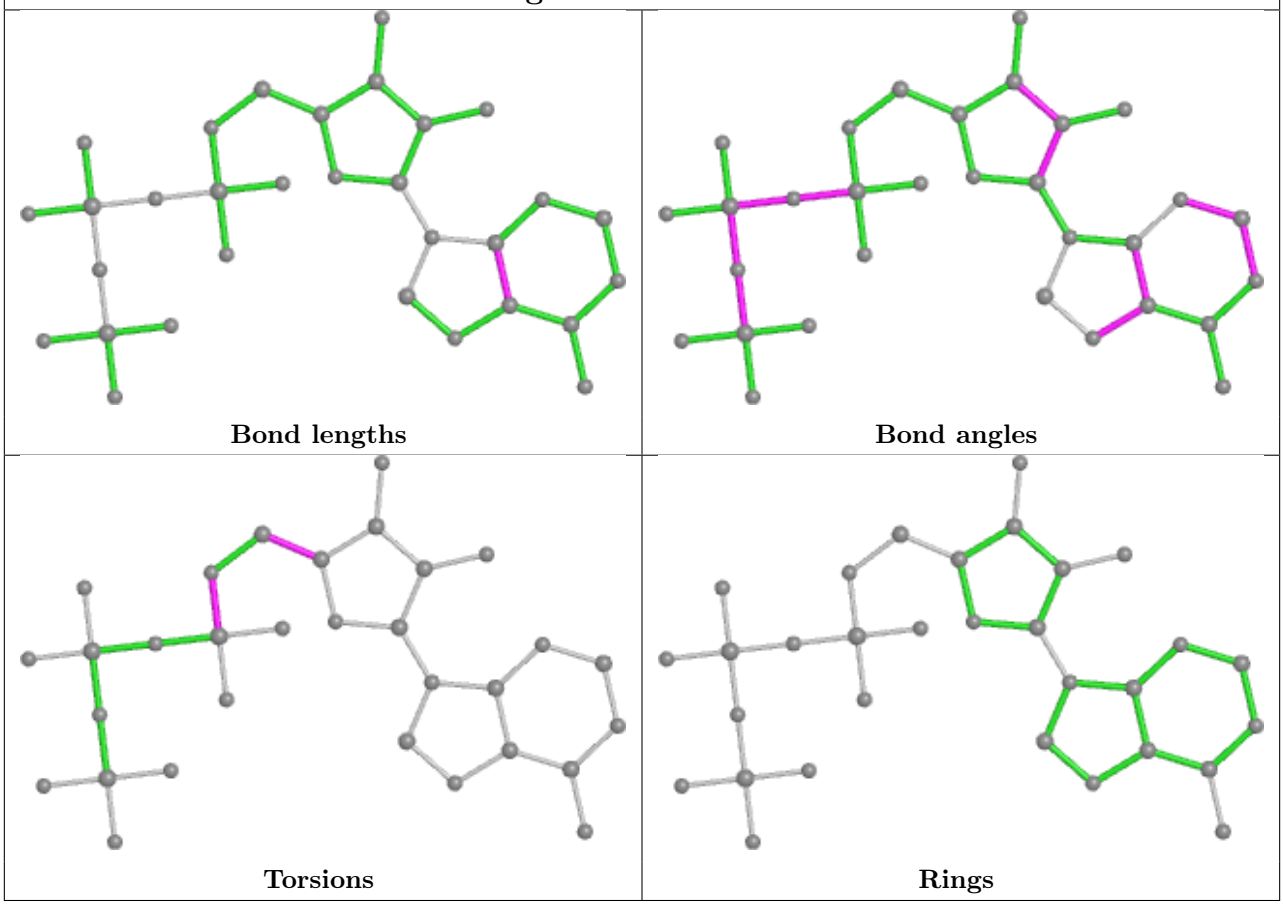
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

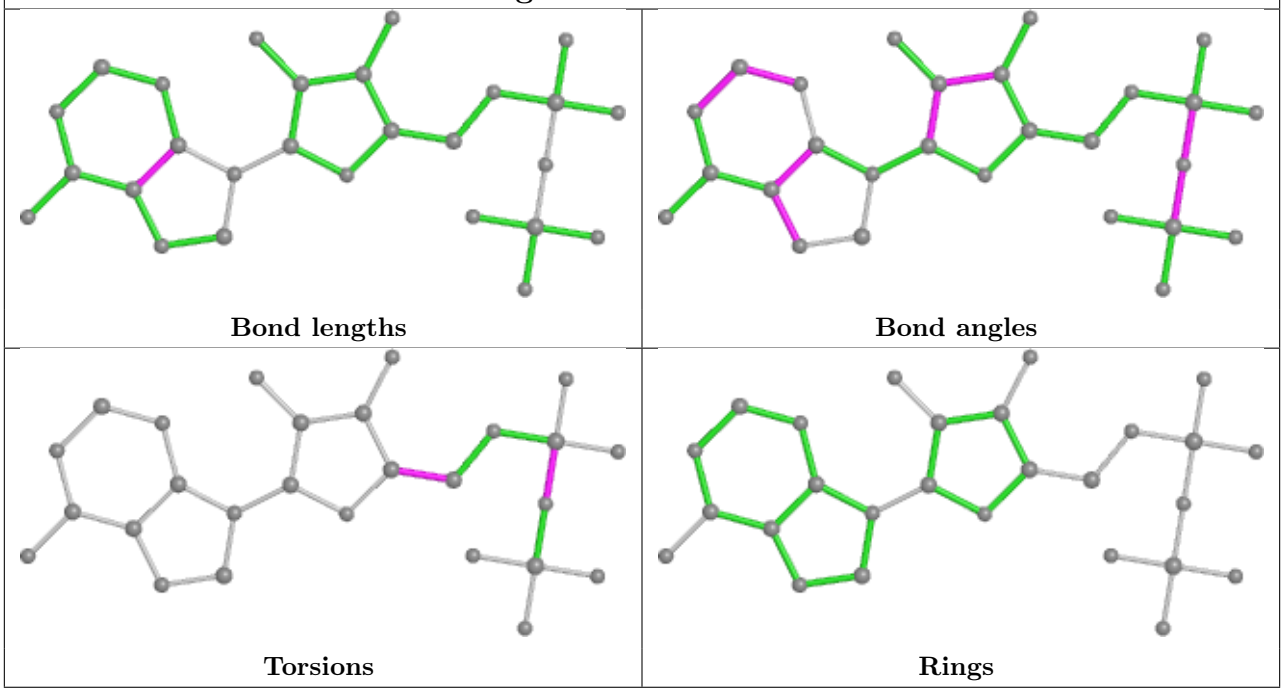
Ligand ATP A 502



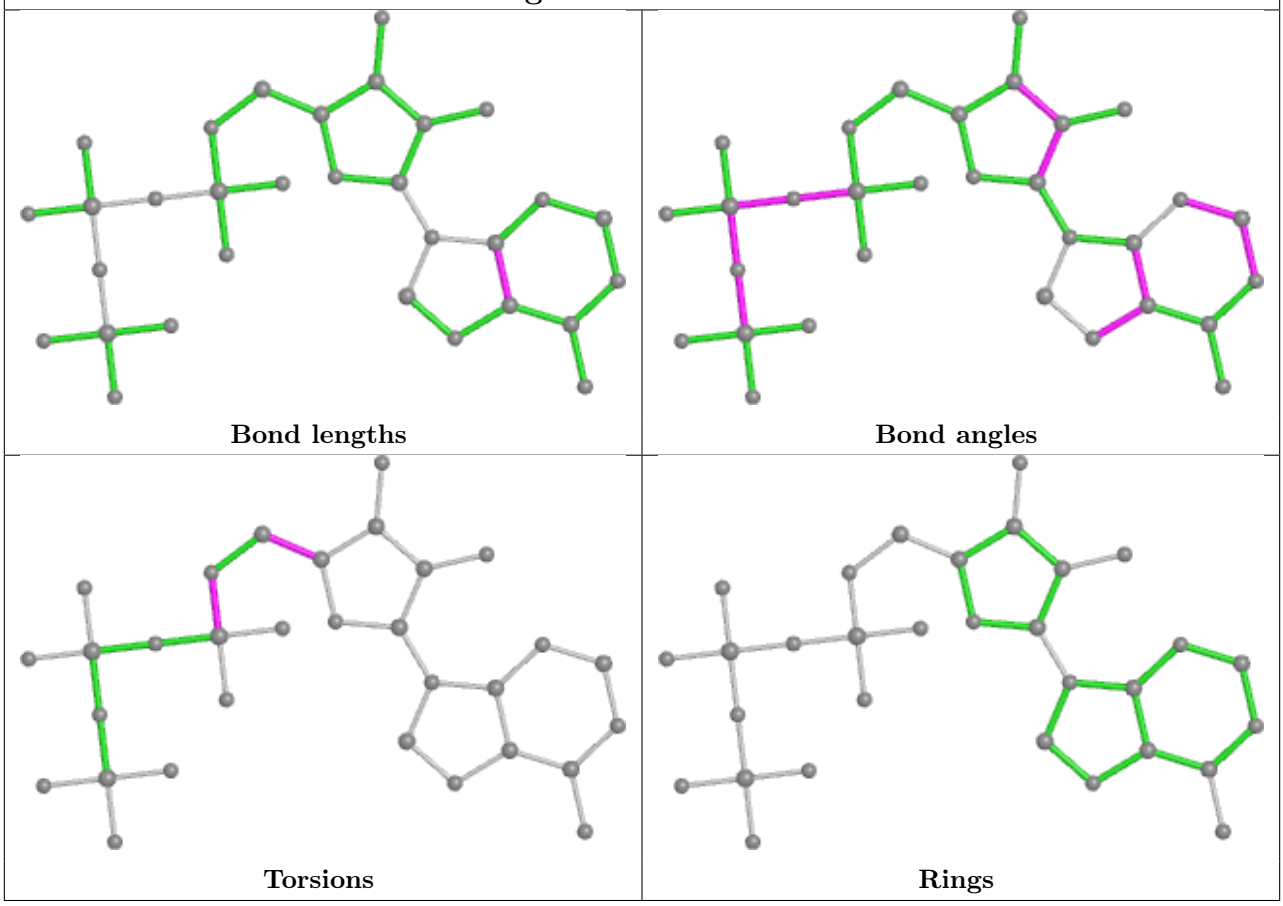
Ligand ATP C 501



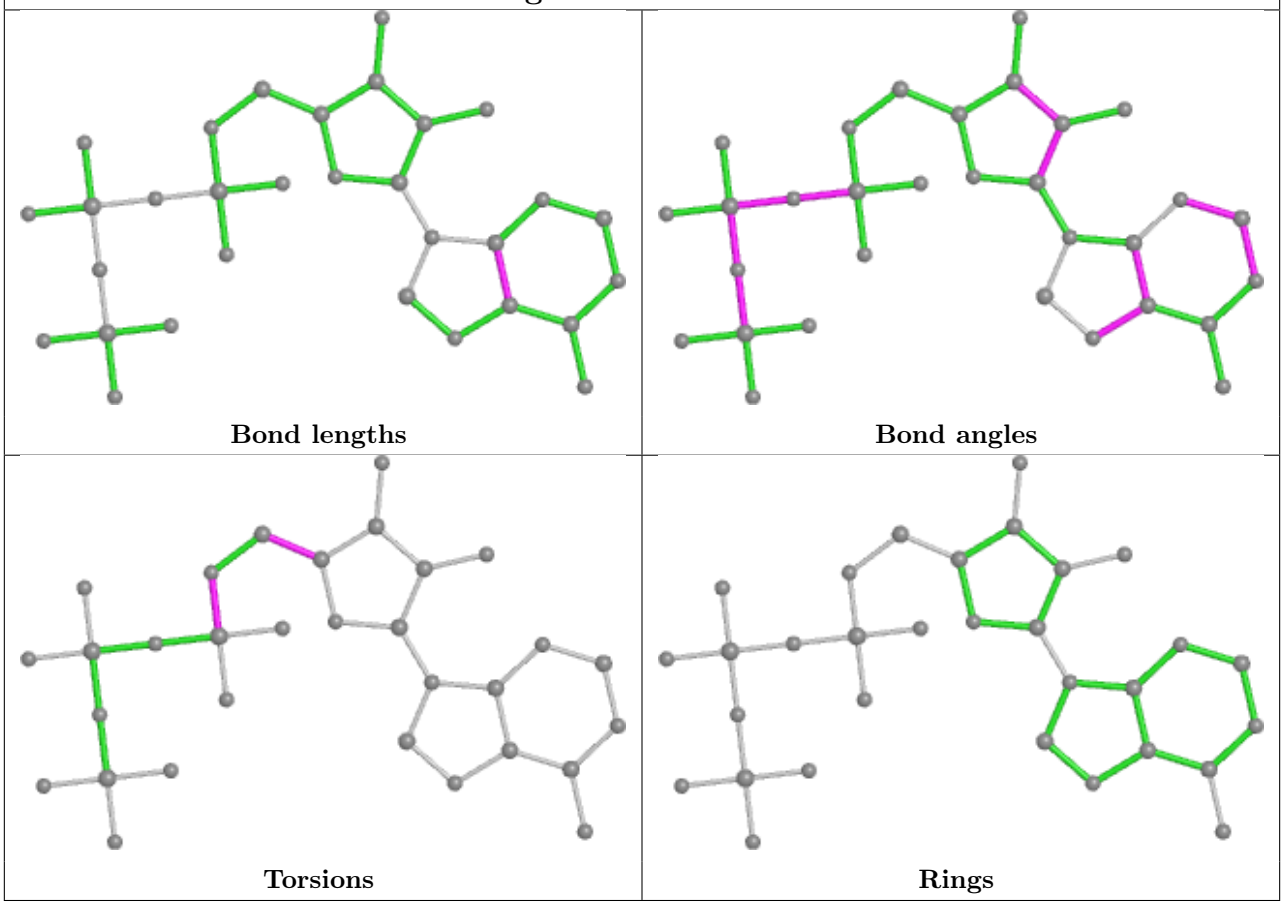
Ligand ADP F 2001



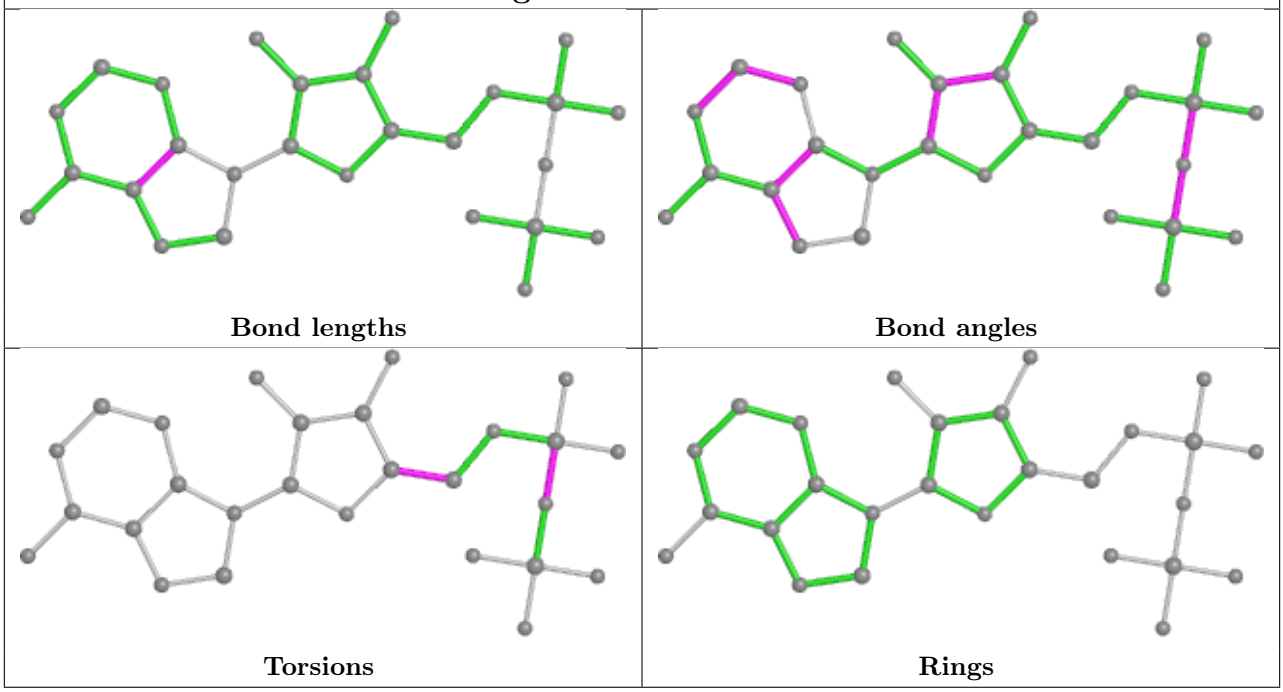
Ligand ATP A 501



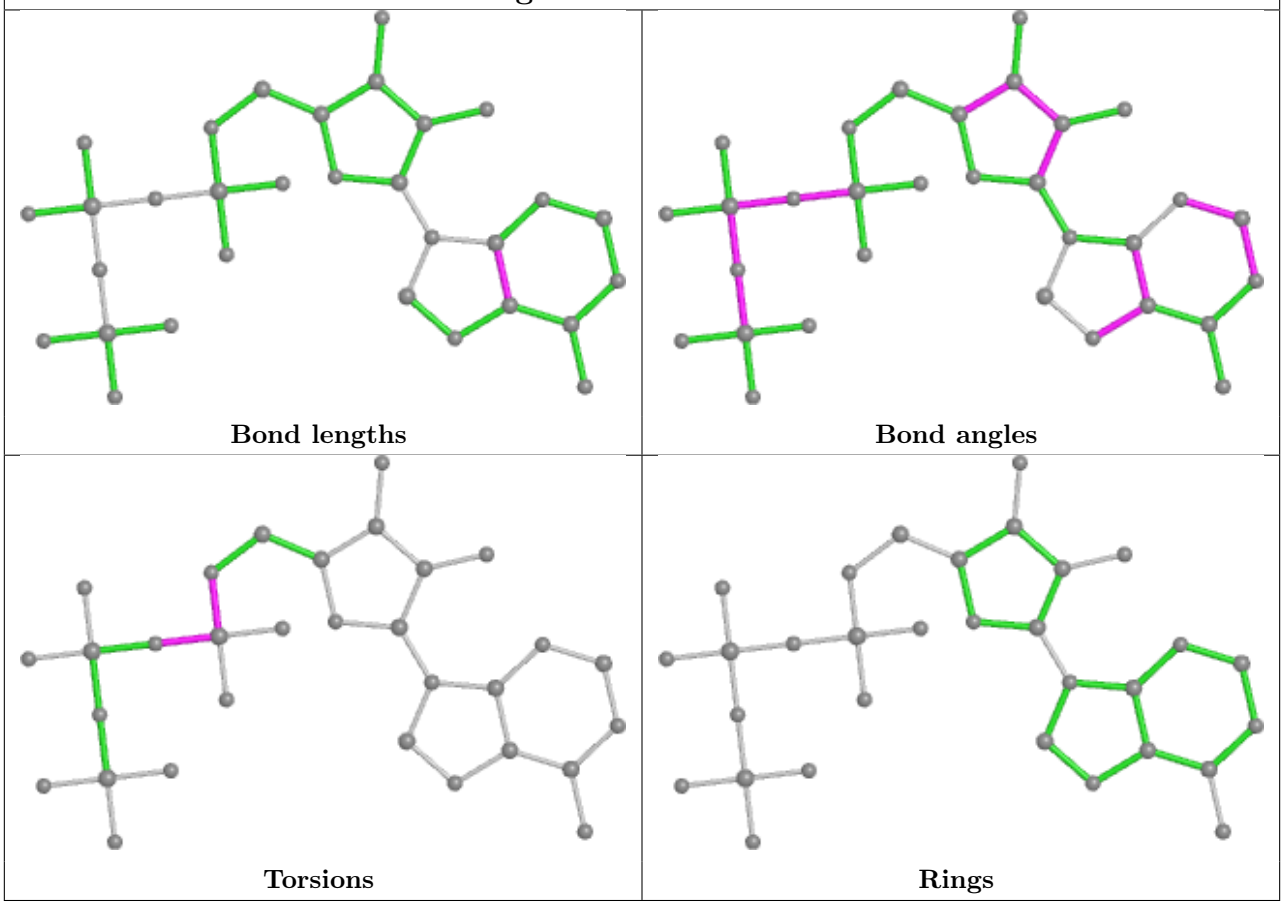
Ligand ATP D 501



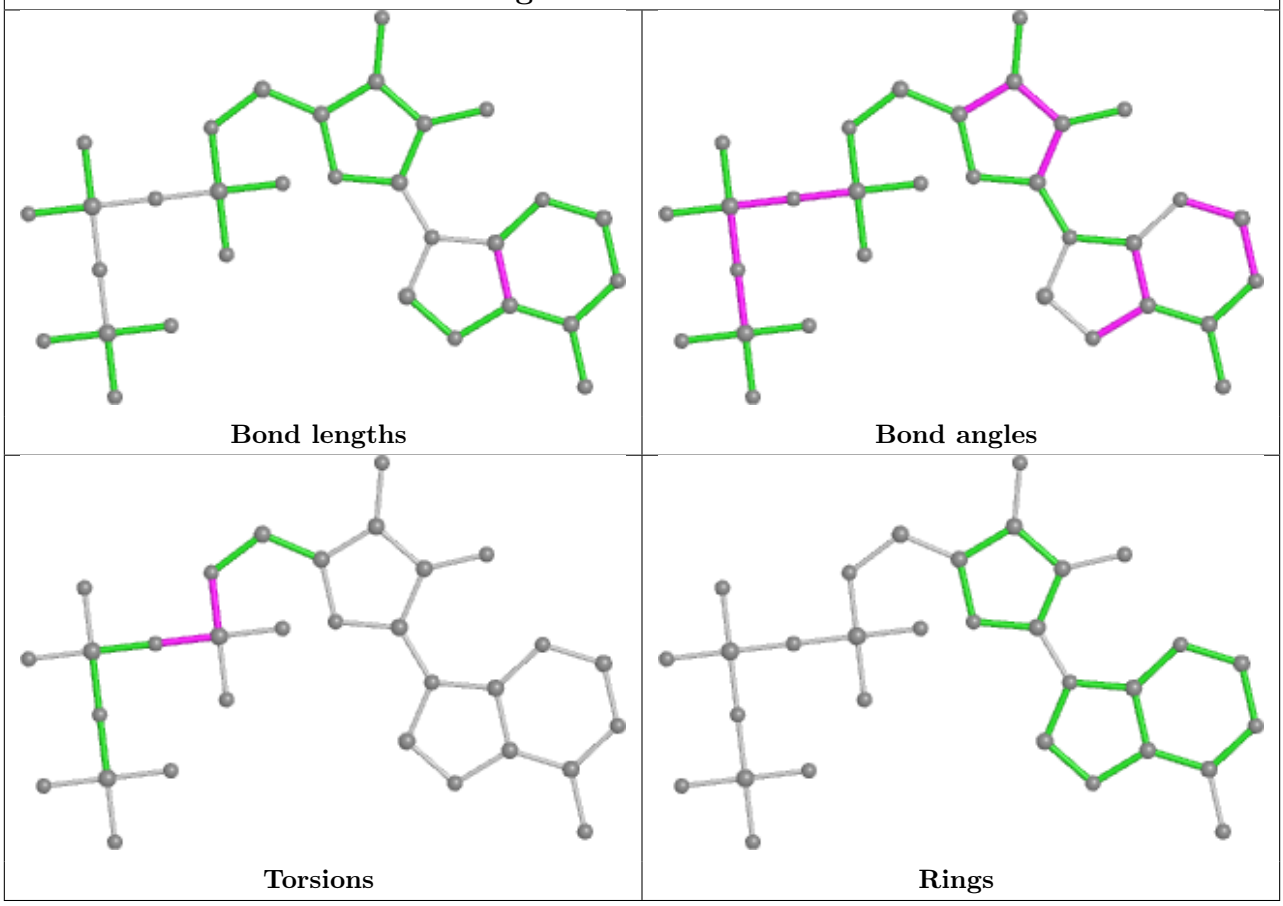
Ligand ADP G 2001



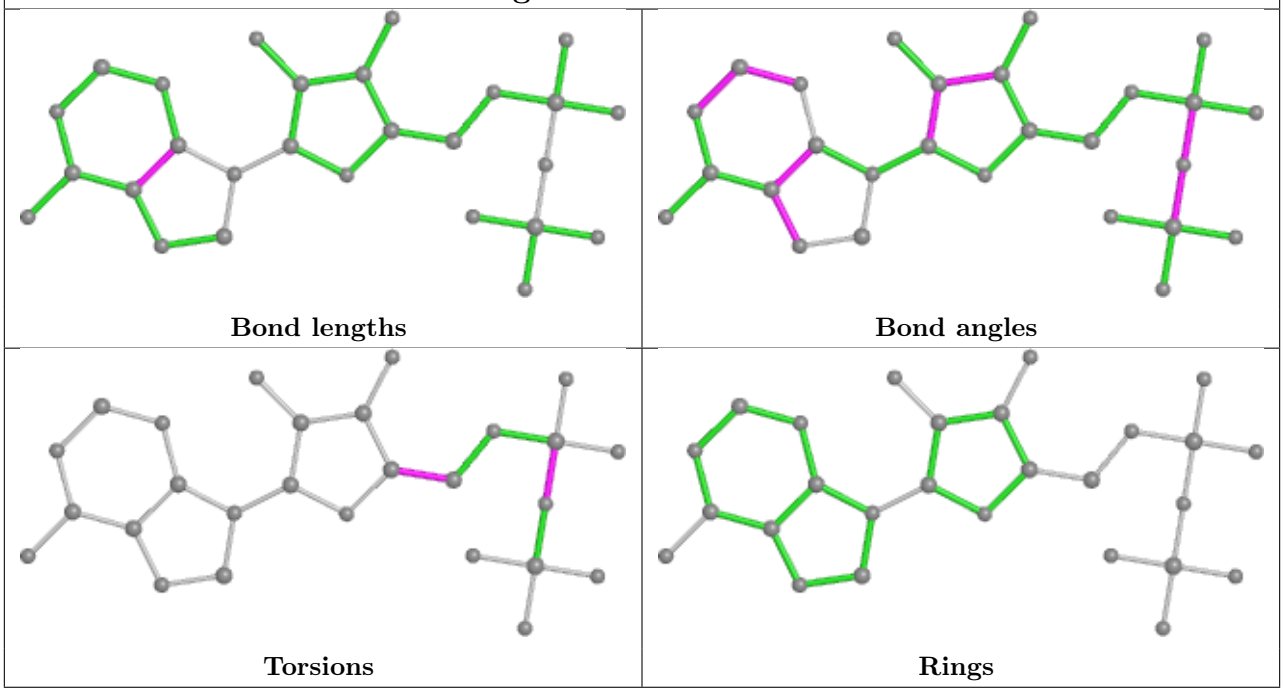
Ligand ATP H 2004



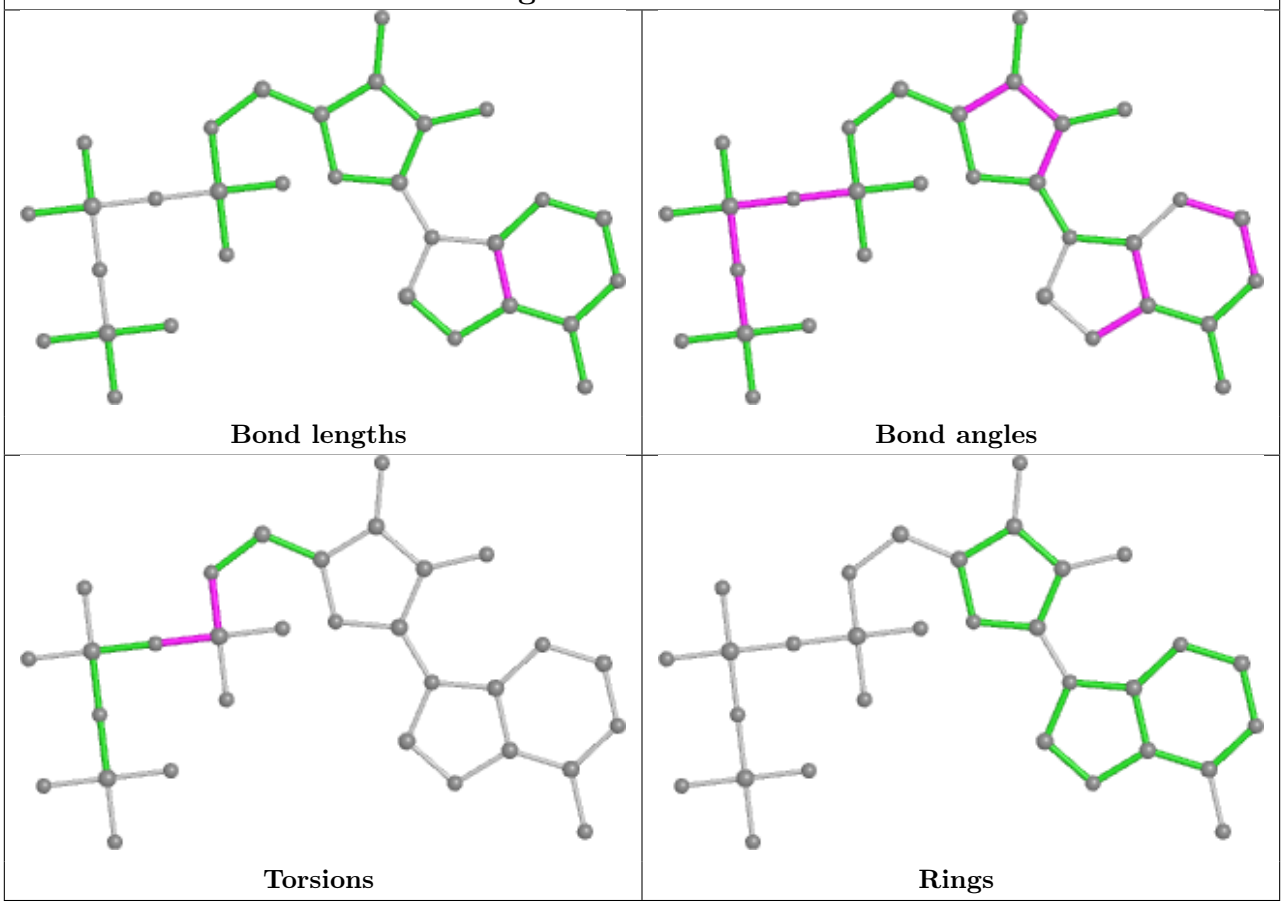
Ligand ATP G 2004



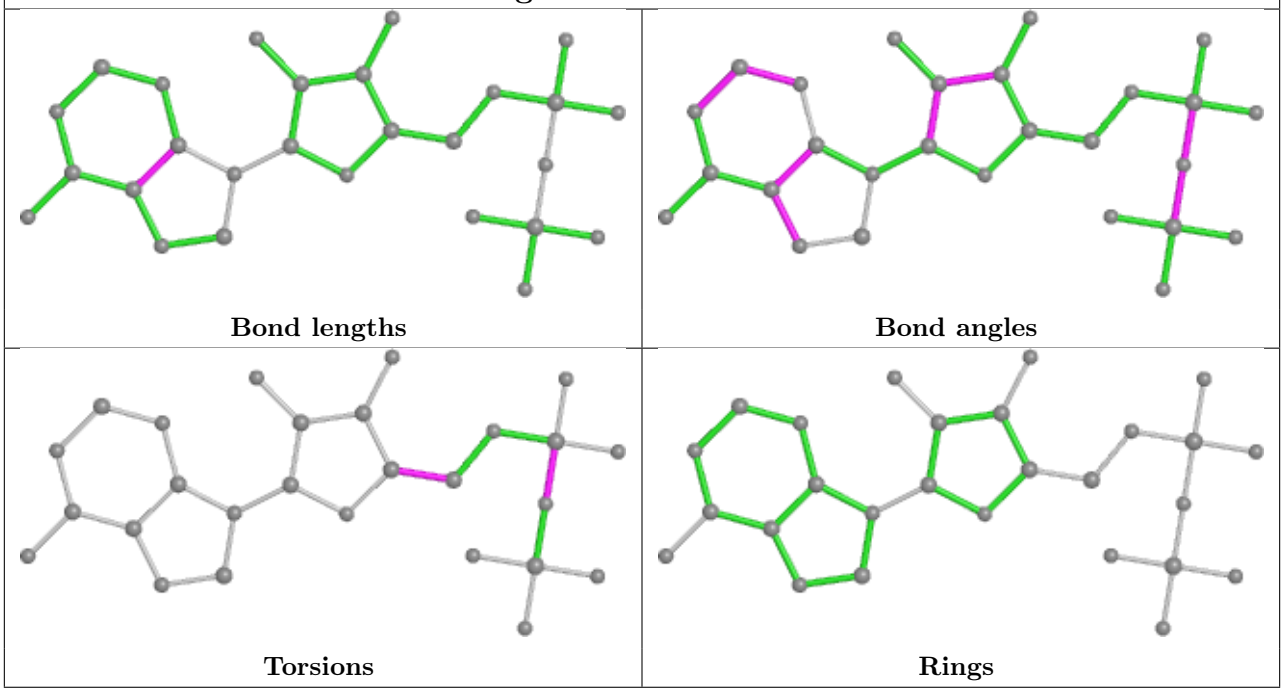
Ligand ADP H 2001



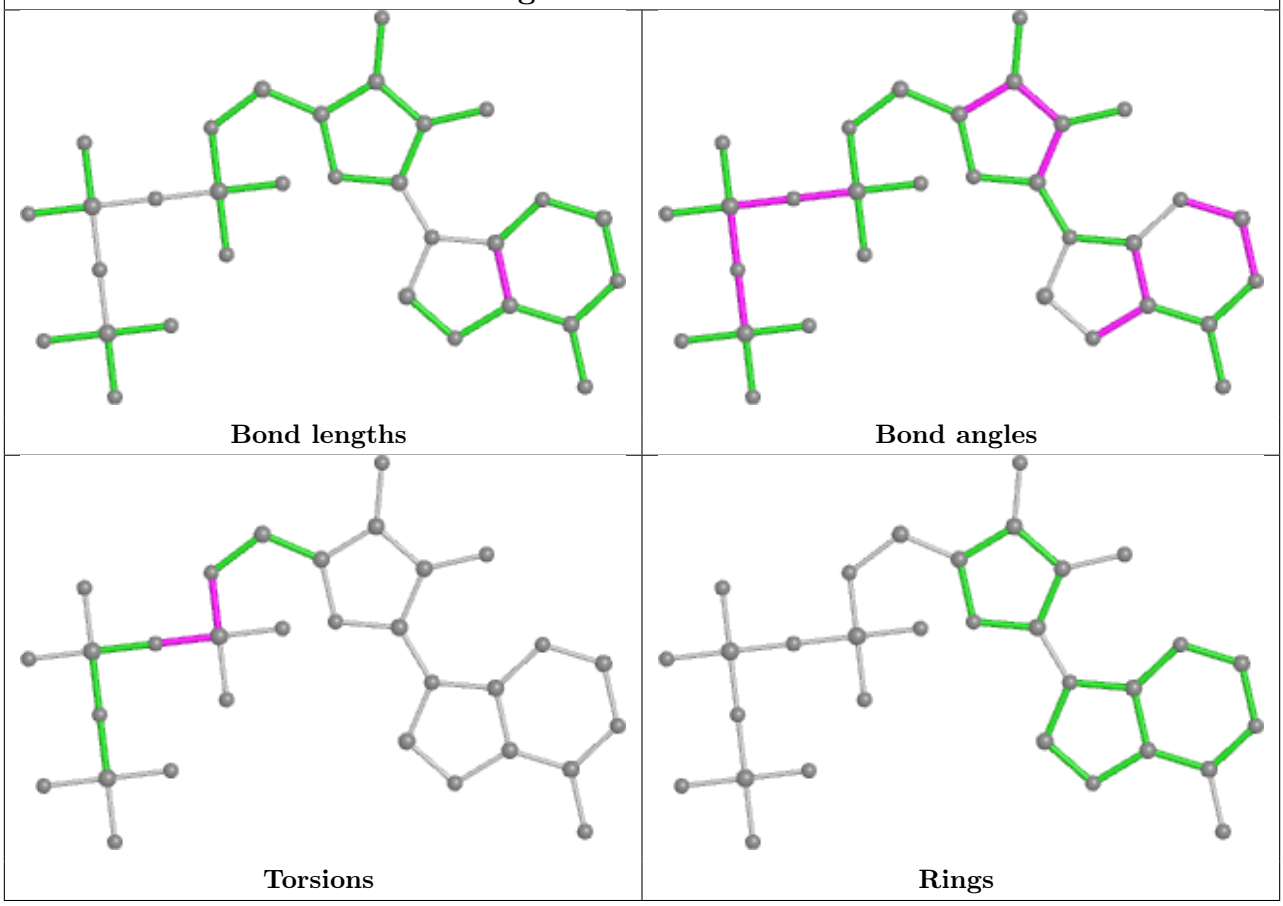
Ligand ATP F 2004



Ligand ADP E 2001



Ligand ATP E 2004



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.

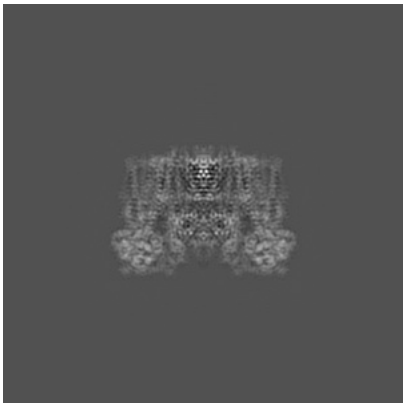
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7339. These allow visual inspection of the internal detail of the map and identification of artifacts.

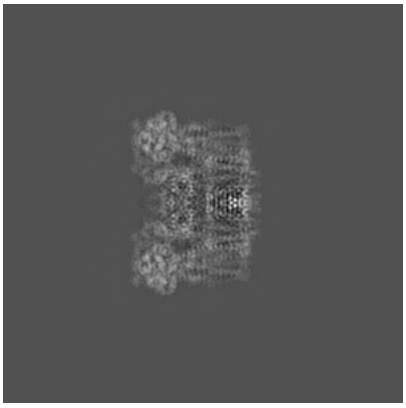
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

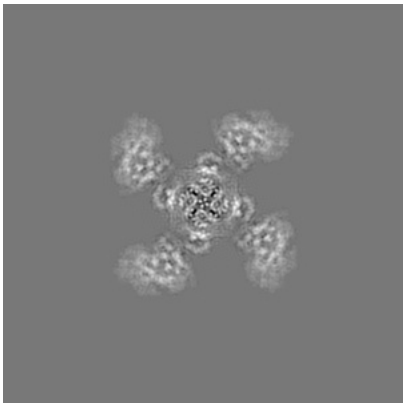
6.1.1 Primary map



X



Y

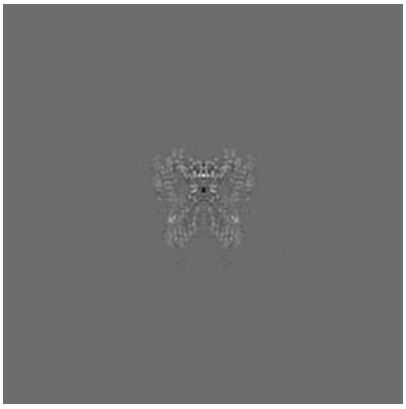


Z

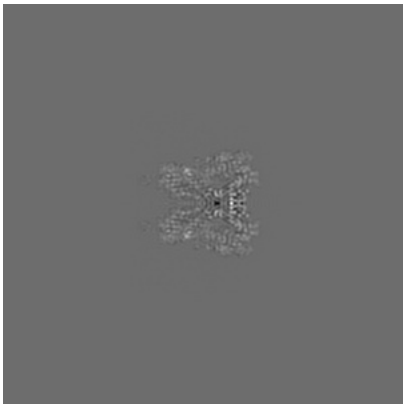
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

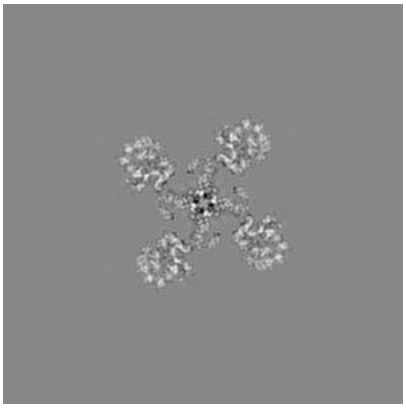
6.2.1 Primary map



X Index: 150



Y Index: 150



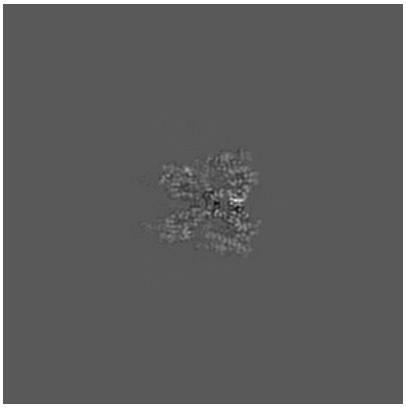
Z Index: 150

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

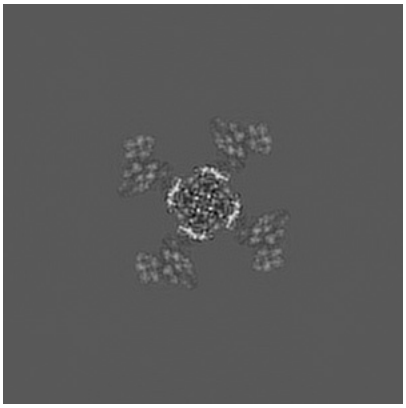
6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 149



Y Index: 149

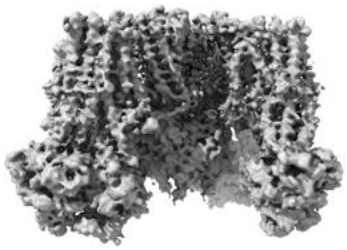


Z Index: 138

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

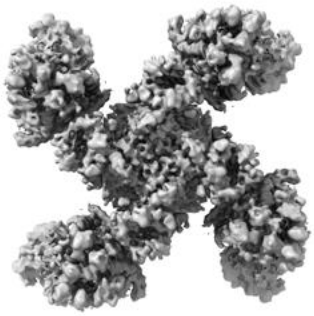
6.4 Orthogonal surface views (i)

6.4.1 Primary map



X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0343. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

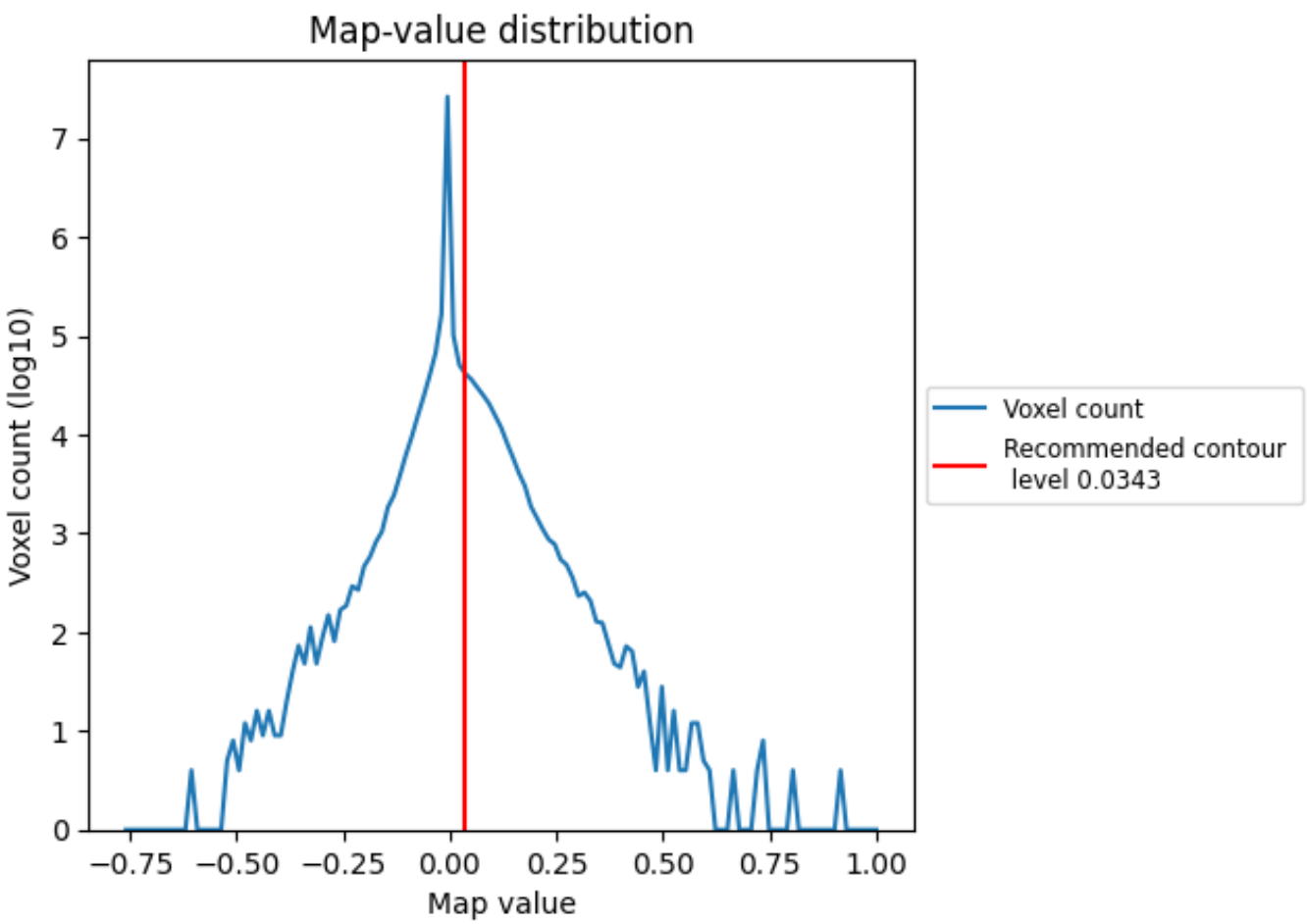
6.5 Mask visualisation (i)

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

7 Map analysis (i)

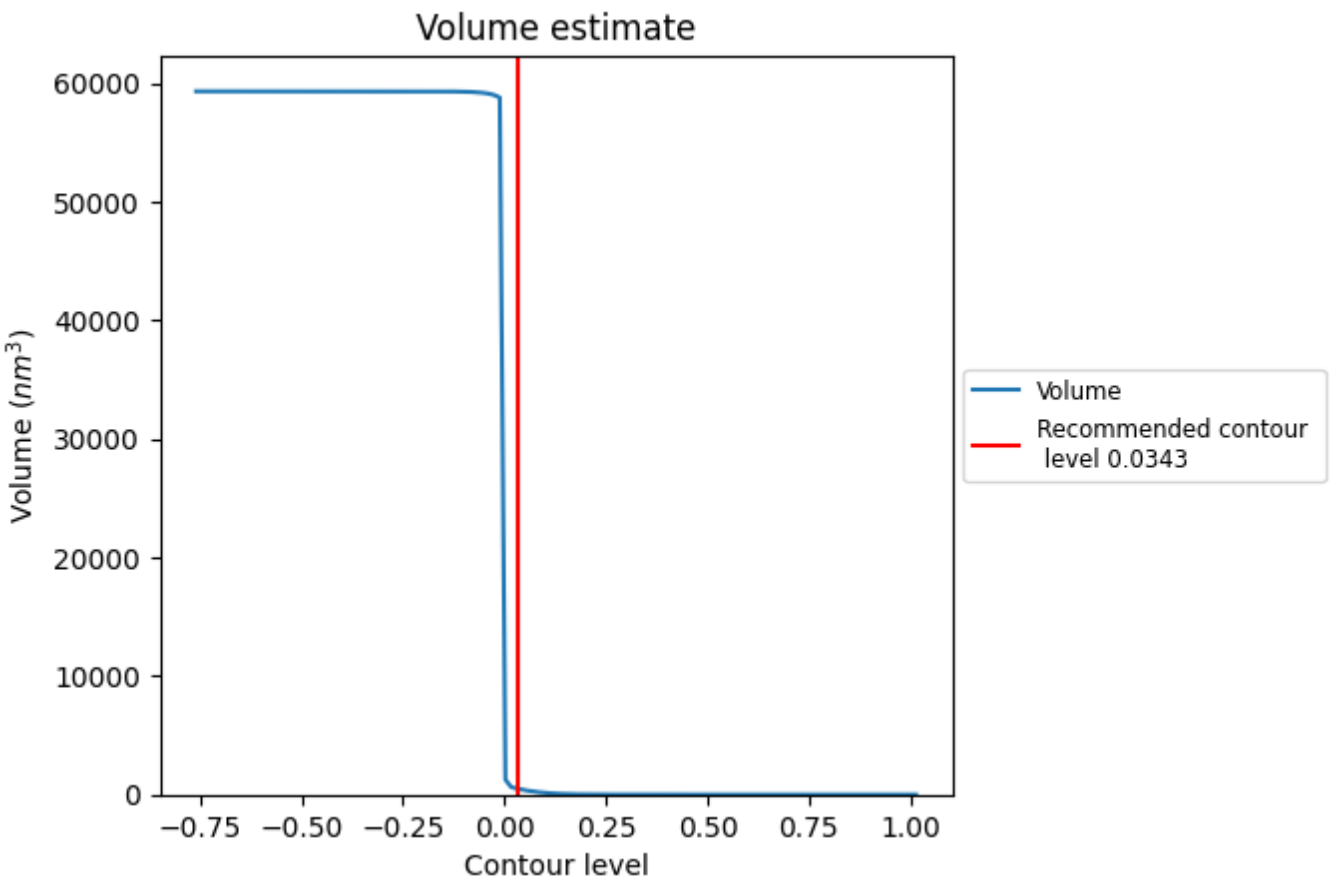
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

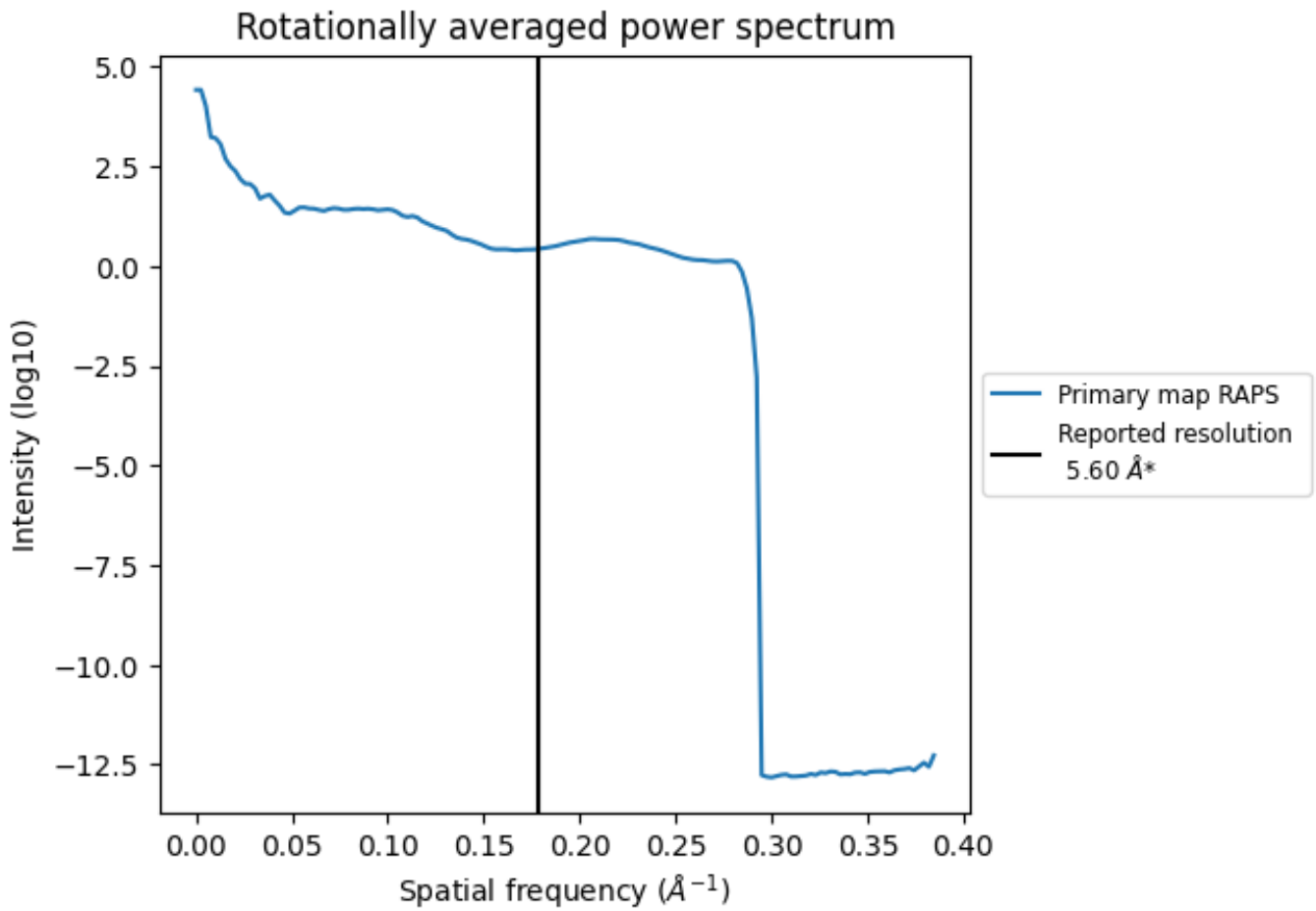
7.2 Volume estimate (i)



The volume at the recommended contour level is 479 nm^3; this corresponds to an approximate mass of 433 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 0.179 Å^{-1}

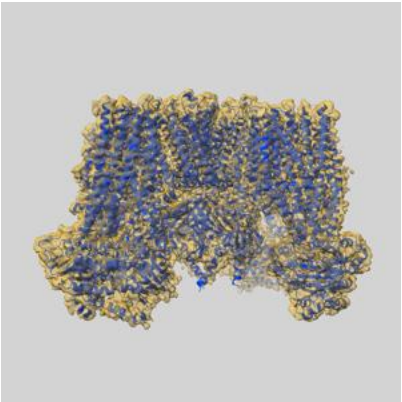
8 Fourier-Shell correlation (i)

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

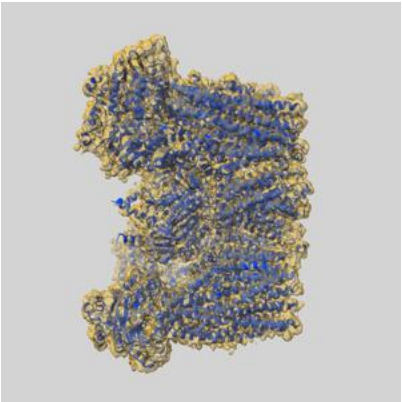
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7339 and PDB model 6C3P. Per-residue inclusion information can be found in section 3 on page 8.

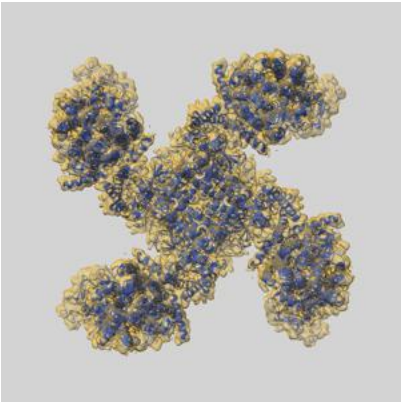
9.1 Map-model overlay (i)



X



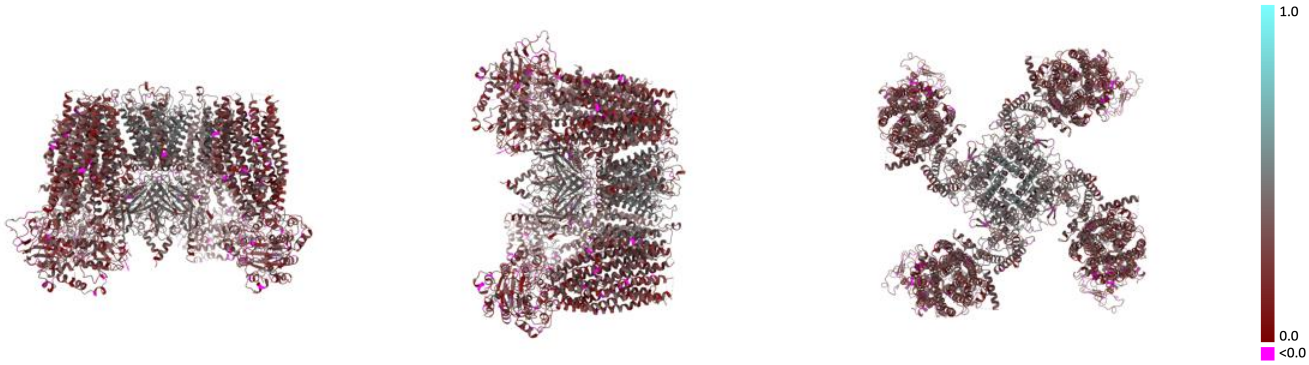
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0343 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.

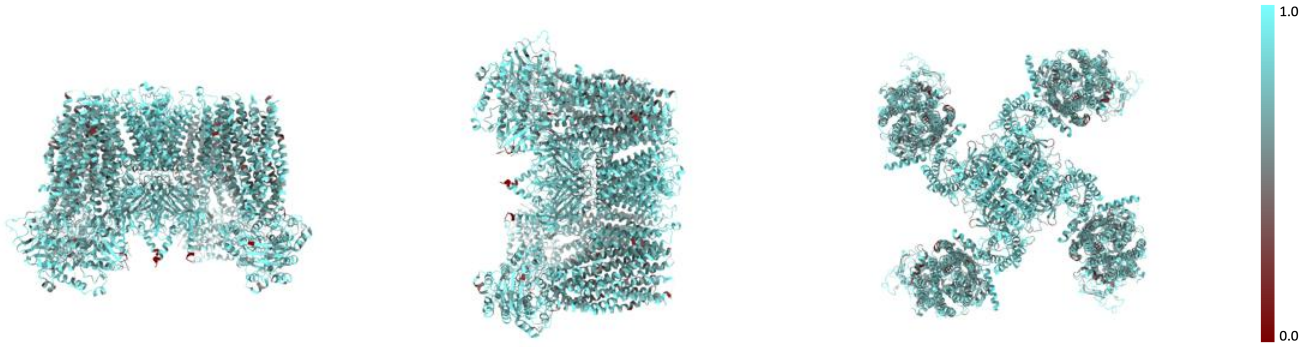
9.2 Q-score mapped to coordinate model (i)



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.

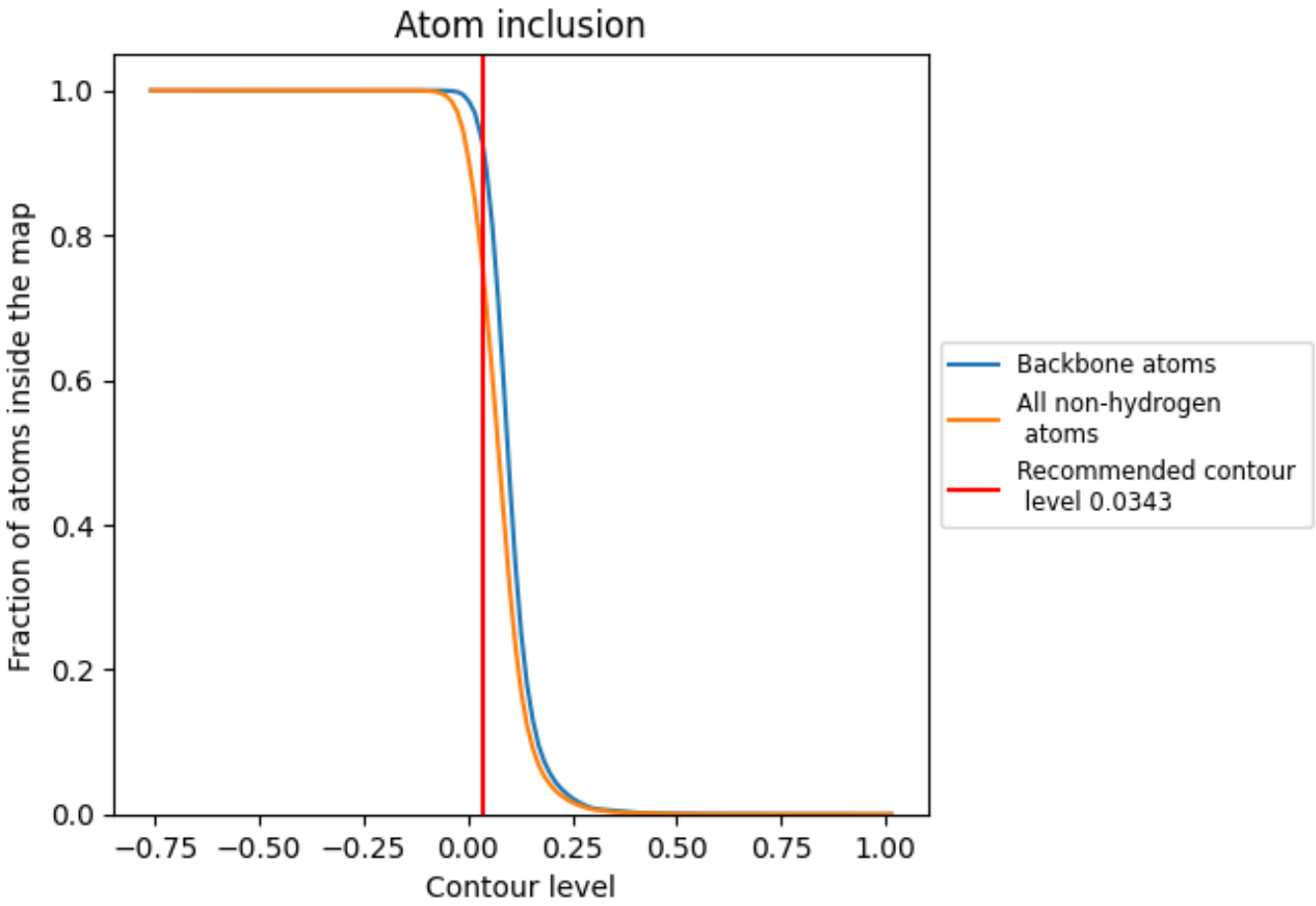
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.0343).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 76% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.0343) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7595	0.2940
A	0.8316	0.3920
B	0.8270	0.3930
C	0.8311	0.3920
D	0.8347	0.3950
E	0.7419	0.2720
F	0.7420	0.2680
G	0.7420	0.2710
H	0.7403	0.2670