



wwPDB/EMDataBank EM Map/Model Validation Summary Report ⓘ

Feb 20, 2018 – 08:32 pm GMT

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/EMDataBank EM Map/Model Validation Summary Report
for a publicly released PDB/EMDB 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 ⓘ symbol.

MolProbity : 4.02b-467
Mogul : 1.7.3 (157068), CSD as539be (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk30686

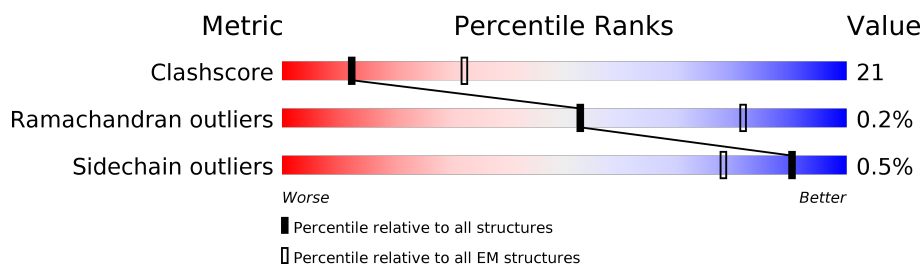
1 Overall quality at a glance

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	136279	1886
Ramachandran outliers	132675	1663
Sidechain outliers	132484	1531

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

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	53% 32% 14%
2	H	1581	53% 32% 14%

2 Entry composition

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
1	A	328	Total	C	N	O	S	0	0
			2506	1619	428	442	17		
1	D	328	Total	C	N	O	S	0	0
			2506	1619	428	442	17		
1	B	328	Total	C	N	O	S	0	0
			2506	1619	428	442	17		
1	C	328	Total	C	N	O	S	0	0
			2506	1619	428	442	17		

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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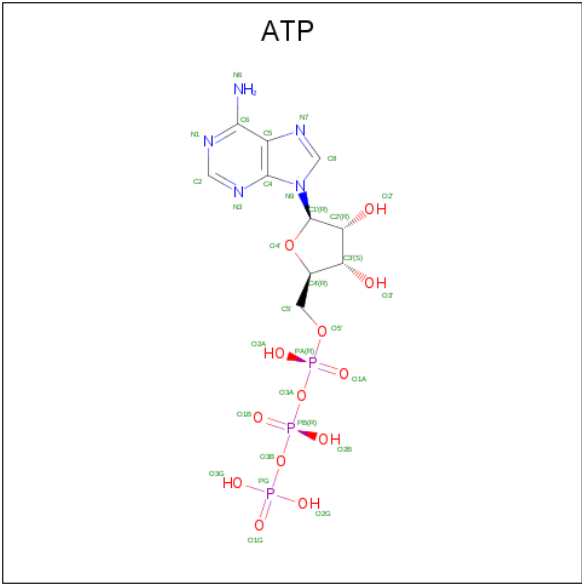
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Chain	Residue	Modelled	Actual	Comment	Reference
D	391	SER	-	expression tag	UNP Q14654
D	392	ASN	-	expression tag	UNP Q14654
D	393	SER	-	expression tag	UNP Q14654
D	394	LEU	-	expression tag	UNP Q14654
D	395	GLU	-	expression tag	UNP Q14654
D	396	VAL	-	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
2	E	1359	Total	C	N	O	S	0	0
			10077	6567	1699	1760	51		
2	H	1359	Total	C	N	O	S	0	0
			10077	6567	1699	1760	51		
2	G	1359	Total	C	N	O	S	0	0
			10077	6567	1699	1760	51		
2	F	1359	Total	C	N	O	S	0	0
			10077	6567	1699	1760	51		

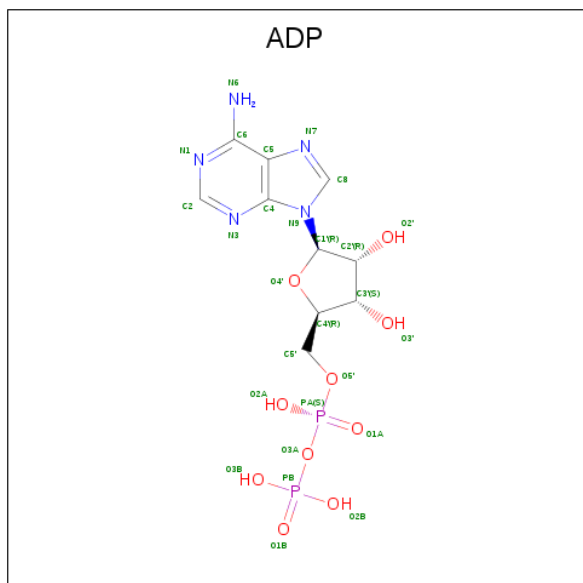
- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



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

- 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
4	E	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	H	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	G	1	Total	C	N	O	P	0
			27	10	5	10	2	
4	F	1	Total	C	N	O	P	0
			27	10	5	10	2	

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

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

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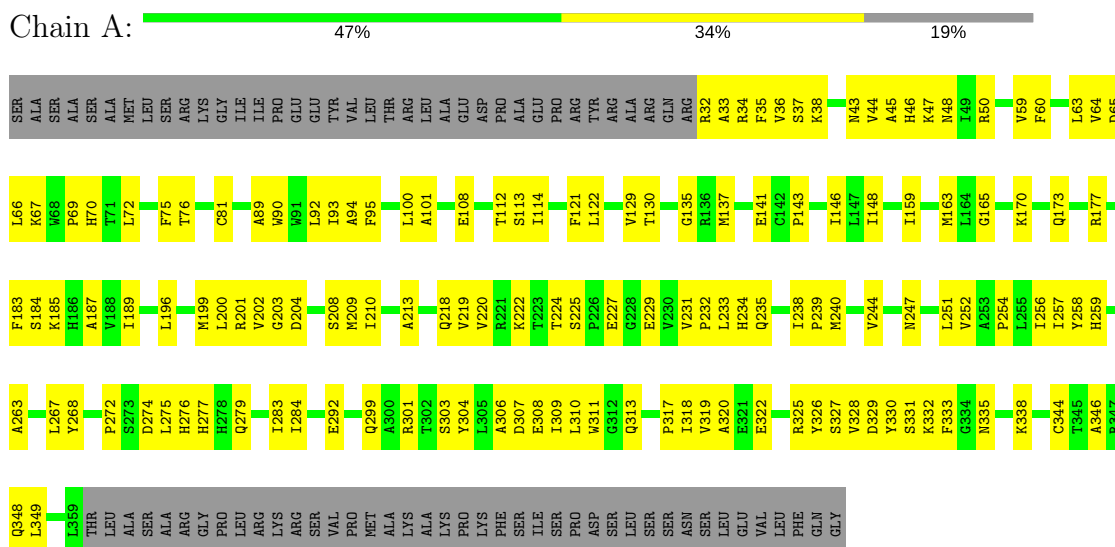
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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	E	2	2	2	0

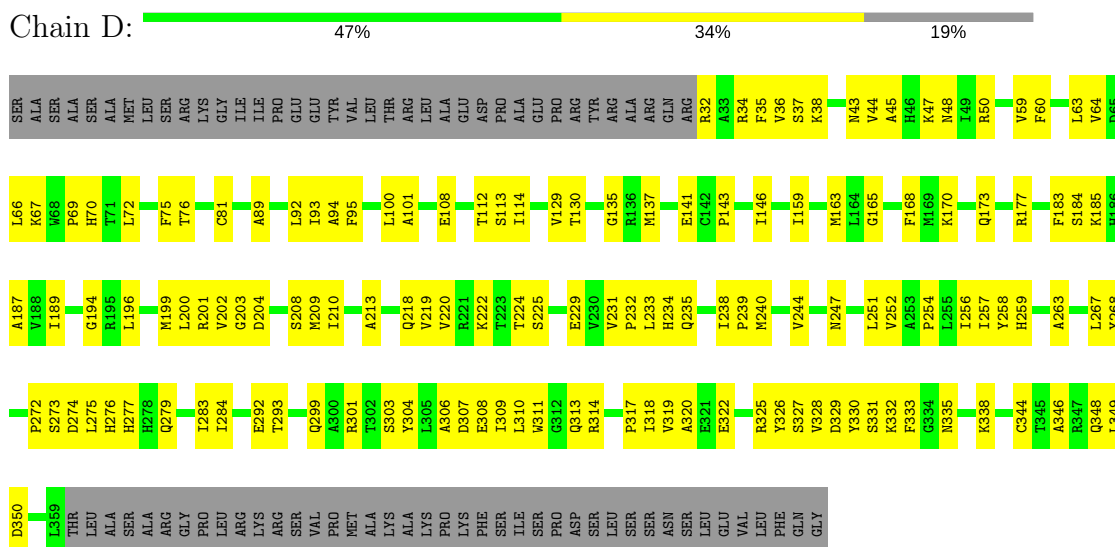
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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

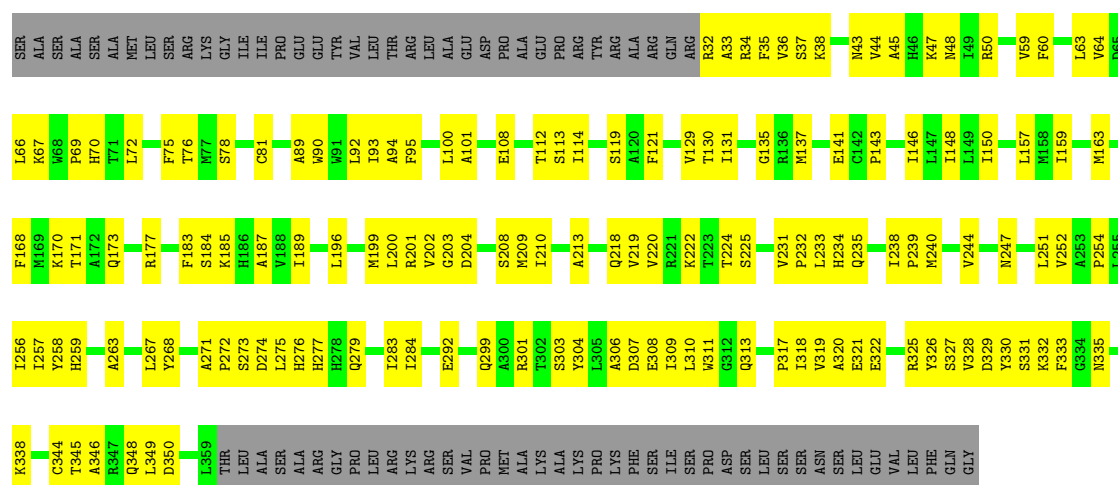


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



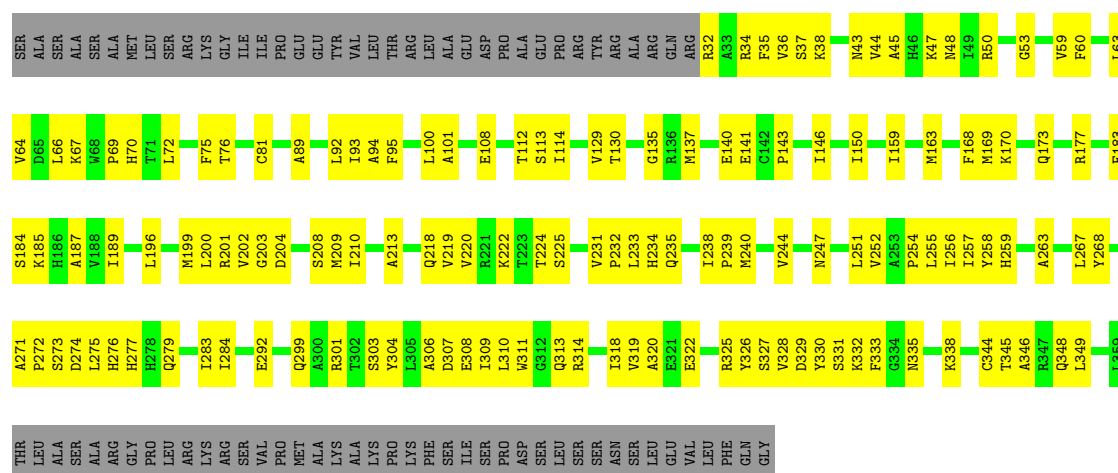
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain B: 



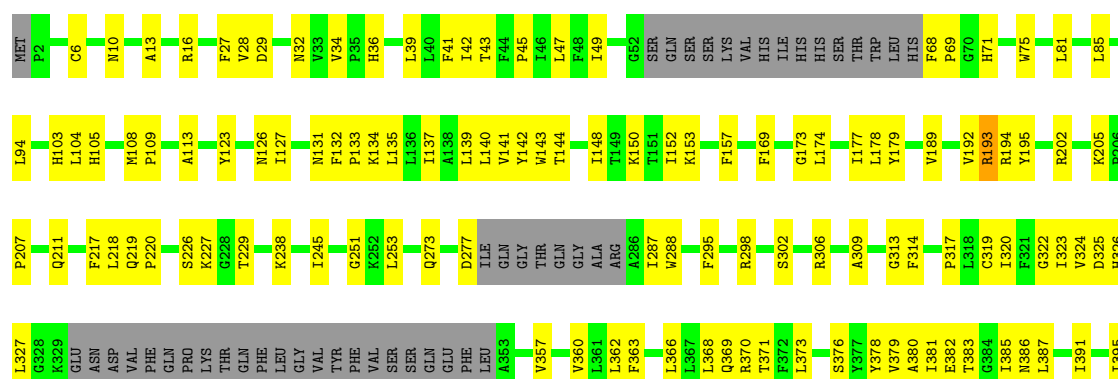
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

Chain C: 



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

Chain E: 

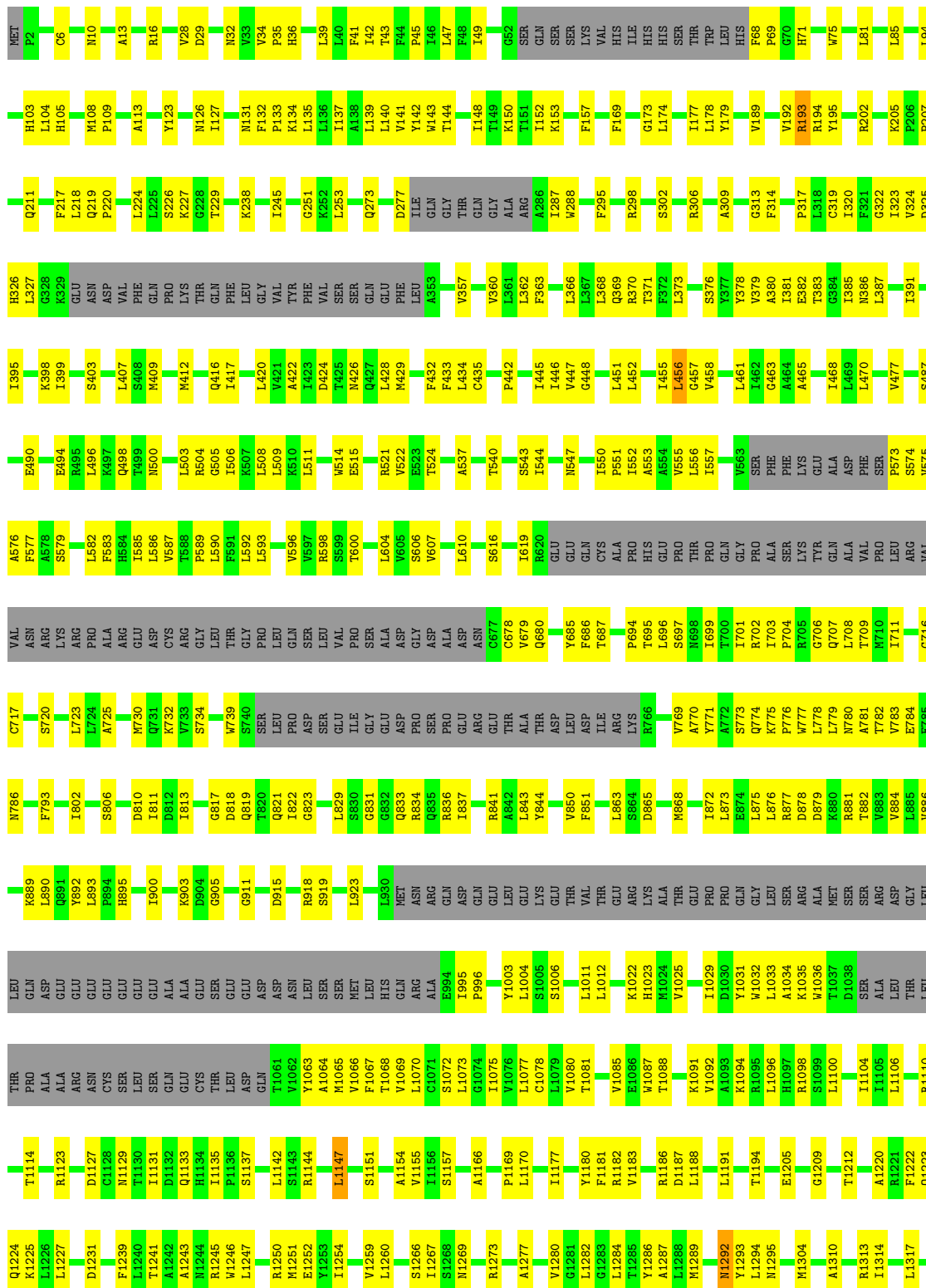


VAL	PRO	PHE	V477	K398
LEU	ASP	SER	S487	1399
ARG	SS73			S403
VAL	V575	A576	E490	L407
ASN	F577		E494	S408
ARG	A578		R495	L409
LYS	S579		K497	L496
PRO	L582		L724	N412
ALA	F583		T499	Q416
GLU	H584		N500	L417
ASP	L585		L503	L420
CYS	L586		R504	V421
ARG	V587		G505	A422
GLY	P589		I506	L423
LEU	L590		K507	D424
THR	F591		L508	T425
PRO	L592		L509	N426
LEU	L593		L511	Q427
GLN	V596		W514	L428
SER	N597		E515	F432
LEU	R598		R519	F433
VAL	S599		T520	L434
PRO	T600		R521	C435
ILE	L604		V522	W439
GLY	A605		T524	P442
ASP	S606		A537	L445
ASP	V607		T540	L446
ALA	L610		S543	V447
ASN	S616		I544	G448
C677	C678		N547	L451
V679	V679		GLU	L452
Q690	R620		GLN	T455
Y685	GLU		CYS	P551
F686	GLN		ALA	L456
T687			PRO	G457
P694	P694		HIS	V458
T695	T695		GLU	A554
L696	L696		PRO	V555
S697	S697		THR	L462
N698	N698		PRO	G463
I699	I699		GLN	A464
T700	T700		GLY	A465
I701	I701		PRO	SER
R702	R702		ALA	PHE
I703	I703		LYS	L469
Q704	Q704		LYS	L470
R705	R705		G706	A471
Q706	Q706		THR	ALA
G707	G707		ALA	P472
L708	L708			
I711	I711			
G716	G716			
C717	C717			
S720	S720			
L723	L723			
A725	A725			
W730	W730			
Q731	Q731			
K732	K732			
V733	V733			
S734	S734			
F738	F738			
W739	W739			
SER	SER			
LEU	LEU			
PRO	PRO			
ASP	ASP			
SER	SER			
GLU	GLU			
ILE	ILE			
GLY	GLY			
ALA	ALA			
ASP	ASP			
PRO	PRO			
GLU	GLU			
ARG	ARG			
GLU	GLU			
THR	THR			
ALA	ALA			
THR	THR			
LEU	LEU			
ASP	ASP			
ASN	ASN			
C677	C678			
V679	V679			
Q690	Q690			
Y685	Y685			
F686	F686			
T687	T687			
P694	P694			
T695	T695			
L696	L696			
S697	S697			
N698	N698			
I699	I699			
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I701	I701			
R702	R702			
I703	I703			
Q704	Q704			
R705	R705			
Q706	Q706			
G707	G707			
L708	L708			
I711	I711			
G716	G716			
C717	C717			
S720	S720			
L723	L723			
A725	A725			
W730	W730			
Q731	Q731			
K732	K732			
V733	V733			
S734	S734			
F738	F738			
W739	W739			
SER	SER			
LEU	LEU			
PRO	PRO			
ASP	ASP			
SER	SER			
GLU	GLU			
ILE	ILE			
GLY	GLY			
ALA	ALA			
ASP	ASP			
PRO	PRO			
GLU	GLU			
ARG	ARG			
GLU	GLU			
THR	THR			
ALA	ALA			
THR	THR			
LEU	LEU			
ASP	ASP			
ASN	ASN			
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V679	V679			
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N698	N698			
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LEU	LEU			
PRO	PRO			
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SER	SER			
GLU	GLU			
ILE	ILE			
GLY	GLY			
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THR	THR			
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V733	V733			
S734	S734			
F738	F738			
W739	W739			
SER	SER			
LEU	LEU			
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GLU	GLU			
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GLU	GLU			
THR	THR			
ALA	ALA			
THR	THR			
LEU	LEU			
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ASN	ASN			
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V679	V679			
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F686	F686			
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I703	I703			
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V733	V733			
S734	S734			
F738	F738			
W739	W739			
SER	SER			
LEU	LEU			
PRO	PRO			
ASP	ASP			
SER	SER			
GLU	GLU			
ILE	ILE			
GLY	GLY			
ALA	ALA			
ASP	ASP			
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GLU	GLU			
ARG	ARG			
GLU	GLU			
THR	THR			
ALA	ALA			
THR	THR			
LEU	LEU			
ASP	ASP			
ASN	ASN			
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I711	I711			
G716	G716			
C717	C717			
S720	S720			
L723	L723			
A725	A725			
W730	W730			
Q731	Q731			
K732	K732			
V733	V733			
S734	S734			
F738	F738			
W739	W739			
SER	SER			
LEU	LEU			
PRO	PRO			
ASP	ASP			
SER	SER			
GLU	GLU			
ILE	ILE			
GLY	GLY			
ALA	ALA			
ASP	ASP			
PRO	PRO			
GLU	GLU			
ARG	ARG			
GLU	GLU			
THR	THR			
ALA	ALA			
THR	THR			
LEU	LEU			
ASP	ASP			
ASN	ASN			
C677	C678			
V679	V679			
Q690	Q690			
Y685	Y685			
F686	F686			
T687	T687			
P694	P694			
T695	T695			

Q1520	T1416	P1339	K1225	R1123	ALA	ASP	L890	I787	S720	F577	E490	K388	L327	Q211	H103
V1523	L1417	D1340	L1226	D1127	ALA	GLU	G891	F793	L723	A578	E494	I399	G528	F217	L104
F1527	S1418	G1342	L1227	C1128	ASN	GLU	L892	L724	L724	S579	E495	L399	K329	L218	H105
T1531	R1419	G1343	D1231	C1129	CYS	GLU	H894	A725	A725	L582	L496	S403	ASN	Q219	M108
I1535	I1424	K1344	F1239	M1129	LEU	GLU	H895	S806	M730	F583	Q498	L407	VAL	P220	P109
P1428	P1428	Q1345	L1240	I1131	SER	GLU	I900	S806	M730	F584	Q498	L407	VAL	L224	A113
V1429	V1429	Q1346	L1241	D1132	GLN	ALA	K903	D810	G731	I585	Q499	M408	PHE	L225	A113
F1431	F1431	M1348	R1245	H1133	GLU	ALA	K904	D811	G732	L586	M500	M409	GLN	S226	Y123
V1538	V1538	L1349	W1246	H1134	CYS	GLU	D904	D812	G733	F587	L503	M412	LYS	K227	Y123
V1539	V1539	S1350	L1247	I1135	THR	SER	G905	I813	S734	F588	L503	M412	LYS	G228	N126
I1542	I1542	R1352	L1247	P1136	LEU	GLU	G911	G817	F738	F589	G505	Q416	GLN	T229	I127
D1546	D1546	P1359	R1250	S1137	ASP	ASP	D915	G818	F739	L592	L506	I417	PHE	K238	N131
L1547	L1547	V1360	M1251	L1142	ASN	ASP	D915	Q819	S740	L593	L508	L420	GLY	K238	N131
V1548	V1548	Y1253	E1252	R1143	LEU	ASN	R918	Q820	S740	L593	L508	L420	GLY	F132	F132
W1451	W1451	K1362	I1254	R1144	GLN	GLN	R919	Q821	S740	L593	L508	L420	GLY	P133	P133
V1550	V1550	H1363	I1254	L1147	ASP	SER	S919	I822	S740	L593	L508	L420	GLY	K134	K134
I1556	I1556	M1365	I1254	L1147	GLN	GLN	S919	I822	S740	L593	L508	L420	GLY	L135	L135
F1559	F1559	L1367	S1266	L1153	GLN	GLN	S919	I822	S740	L593	L508	L420	GLY	G251	G251
D1560	D1560	L1368	I1267	L1153	ASP	ASP	S919	I822	S740	L593	L508	L420	GLY	K252	K252
K1561	K1561	L1368	I1267	L1153	GLN	GLN	S919	I822	S740	L593	L508	L420	GLY	K252	K252
K1569	K1569	L1368	I1267	L1153	GLN	GLN	S919	I822	S740	L593	L508	L420	GLY	K252	K252
K1581	K1581	L1368	I1267	L1153	GLN	GLN	S919	I822	S740	L593	L508	L420	GLY	K252	K252
I1474	I1474	R1379	A1277	P1169	LEU	LEU	L930	S830	S740	L593	L508	L420	GLY	K252	K252
T1475	T1475	F1380	V1280	L1170	GLY	GLY	L930	S830	S740	L593	L508	L420	GLY	K252	K252
G1478	G1478	G1381	G1281	L1170	GLY	GLY	L930	S830	S740	L593	L508	L420	GLY	K252	K252
F1481	F1481	G1383	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
S1482	S1482	K1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
Q1483	Q1483	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
Q1484	Q1484	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
Q1485	Q1485	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
Q1486	Q1486	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
Q1487	Q1487	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
L1488	L1488	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
F1489	F1489	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
C1490	C1490	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
L1491	L1491	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
R1493	R1493	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
A1492	A1492	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
H1401	H1401	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
I1402	I1402	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
I1403	I1403	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
I1501	I1501	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
S1500	S1500	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
M1504	M1504	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
D1505	D1505	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
E1506	E1506	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
A1507	A1507	L1384	L1283	L1177	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
I1511	I1511	P1413	P1335	F1222	THR	THR	L930	S830	S740	L593	L508	L420	GLY	K252	K252
D1512	D1512	H1415	W1338	Q1224	PRO	PRO	L930	S830	S740	L593	L508	L420	GLY	K252	K252

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

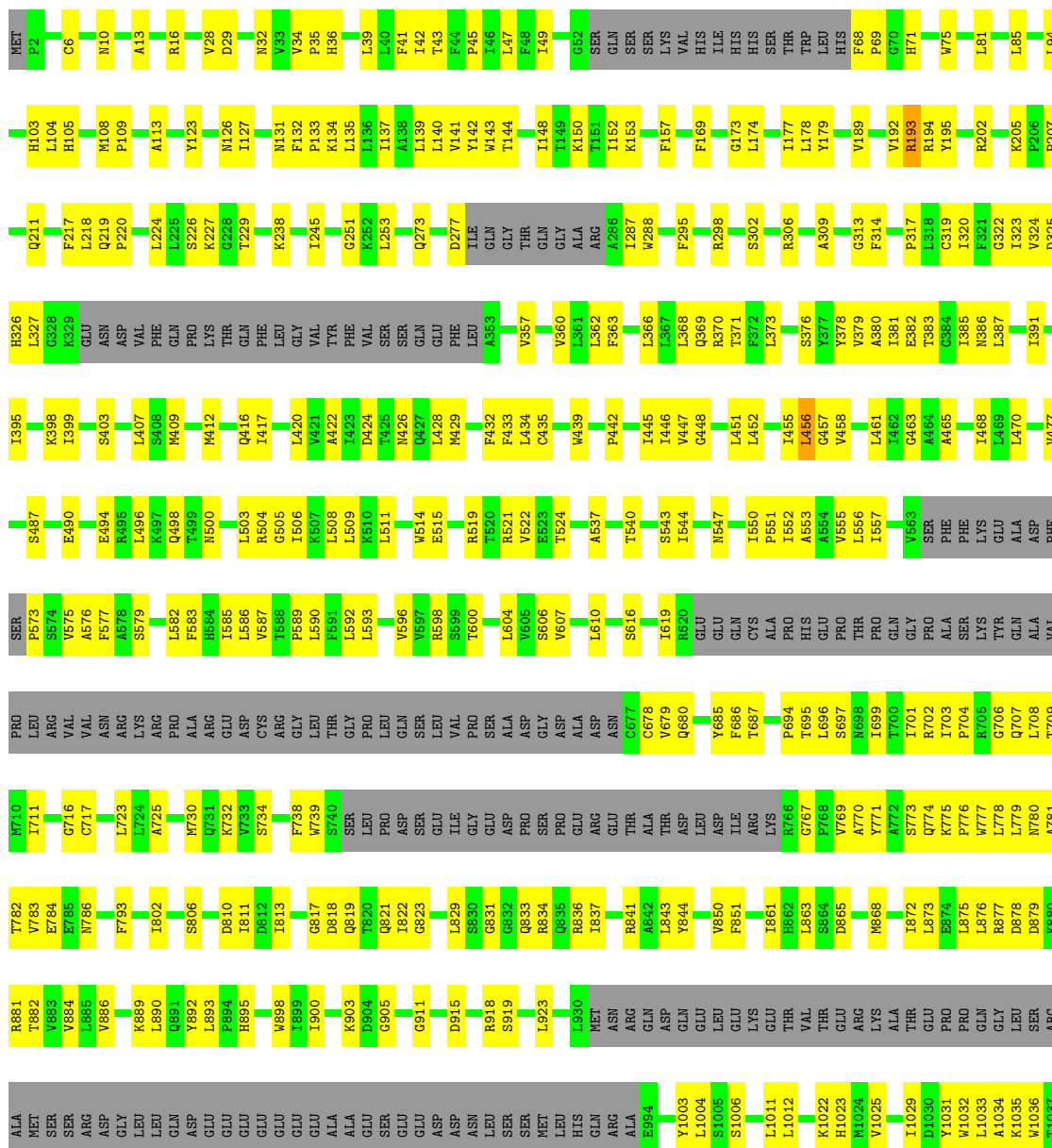
Chain G:





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

Chain F:  53% 32% 14%



D1038	SER	I1104	T1212	L1317	I1402	S1500
	ALA	I1105	A1220	Y1325	I1403	I1501
	LEU	L1106	R1221	F1325	I1404	F1502
	THR		F1222			I1503
	LEU	R1110	Q1223	P1335	I1407	M1504
	THR		Q1224		D1408	I1409
	PRO	T1114	K1225	W1338	I1409	E1506
	ALA		L1226	P1339	P1413	A1507
	ALA	R1123	L1227	D1340		
	ARG			Q1341	T1416	I1511
ASN	D1127	D1231	G1342	R1417	D1512	
CYS	C1128		A1343	L1418		
LEU	M1129	F1239	I1344	I1423	Q1520	
SER	T1130	L1240	Q1345	I1423	V1523	
GLN	I1131	T1241	I1346	I1424		
GLU	D1132		Q1347			
CYS	Q1133	R1245	W1348	V1429	F1527	
THR	H1134	W1246	L1349	L1430		
LEU	I1135	L1247	S1350	F1431	T1531	
ASP	P1136		V1351			
GLN	S1137	R1250	R1352	T1434	I1535	
T1061		M1251	Y1353	I1435		
	L1142	E1252	P1359	M1438	R1538	
	S1143	F1253	L1361		V1539	
	R1144	I1254	K1362	P1441		
		V1259	W1363		I1542	
	L1147	L1260	H1363	W1451	D1546	
			V1364		L1547	
	S1151		M1365	V1459	V1548	
	A1154	I1267	A1366	K1460	I1549	
	V1155	S1268	L1367		V1550	
I1156	M1269	L1368	K1464			
S1157			A1465	I1556		
S1072		R1273	K1373			
L1073			I1374	F1559		
G1074	A1166		G1375	D1560		
I1075	P1169	A1277	I1376	K1561		
L1077	L1170					
C1078		V1280	R1379	L1470		
L1079	I1177	G1281	T1380	D1471		
V1080		L1282	G1381			
T1081	Y1180	L1284	G1383	I1474		
	F1181		K1384	T1475		
R1182		A1287	S1385	G1478		
V1183		L1288	S1386			
		M1289		F1481		
R1186				S1482		
D1187		M1292	L1389	Q1483		
L1188		Y1293		G1484		
K1091		L1294	F1392	Q1485		
V1092		M1295	R1393	R1486		
A1093	L1191		M1394	Q1487		
K1094				L1488		
R1095	T1194	M1304		F1489		
L1096			T1397	C1490		
R1097	E1205	A1310	F1398	L1491		
S1099			E1399	A1492		
L1100	G1209	R1314	W1401	P1493		

4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
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 ($e^-/\text{\AA}^2$)	1.18	Depositor
Minimum defocus (nm)	Not provided	Depositor
Maximum defocus (nm)	Not provided	Depositor
Magnification	Not provided	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
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(°)	Ideal(°)
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(°)	Ideal(°)
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:G:1501:ILE:HG22	2:G:1531:THR:HB	1.55	0.88
2:H:1501:ILE:HG22	2:H: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%)	43	81
1	B	326/406 (80%)	293 (90%)	32 (10%)	1 (0%)	43	81
1	C	326/406 (80%)	293 (90%)	32 (10%)	1 (0%)	43	81
1	D	326/406 (80%)	292 (90%)	33 (10%)	1 (0%)	43	81
2	E	1341/1581 (85%)	1242 (93%)	97 (7%)	2 (0%)	53	88
2	F	1341/1581 (85%)	1241 (92%)	98 (7%)	2 (0%)	53	88
2	G	1341/1581 (85%)	1240 (92%)	99 (7%)	2 (0%)	53	88
2	H	1341/1581 (85%)	1241 (92%)	98 (7%)	2 (0%)	53	88

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	6668/7948 (84%)	6135 (92%)	521 (8%)	12 (0%)	53 85

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 ⓘ

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%)	87 93
2	F	1004/1368 (73%)	998 (99%)	6 (1%)	87 93
2	G	1004/1368 (73%)	998 (99%)	6 (1%)	87 93
2	H	1004/1368 (73%)	998 (99%)	6 (1%)	87 93
All	All	5076/6864 (74%)	5052 (100%)	24 (0%)	90 94

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

Mol	Chain	Res	Type
2	H	1295	ASN
2	G	918	ARG
2	F	1295	ASN
2	H	1379	ARG
2	G	547	ASN

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

Mol	Chain	Res	Type
2	E	1292	ASN
2	H	498	GLN
2	F	926	HIS
2	H	32	ASN
2	H	126	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	501	-	27,33,33	0.96	1 (3%)	27,52,52	2.01	4 (14%)
3	ATP	A	502	-	27,33,33	0.94	1 (3%)	27,52,52	2.04	4 (14%)
3	ATP	C	501	-	27,33,33	0.96	1 (3%)	27,52,52	2.02	4 (14%)
3	ATP	D	501	-	27,33,33	0.95	1 (3%)	27,52,52	2.01	4 (14%)
4	ADP	E	2001	5	25,29,29	0.98	1 (4%)	25,45,45	1.83	3 (12%)
3	ATP	E	2004	5	27,33,33	0.97	1 (3%)	27,52,52	1.96	5 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ADP	F	2001	5	25,29,29	1.00	1 (4%)	25,45,45	1.83	3 (12%)
3	ATP	F	2004	5	27,33,33	1.00	1 (3%)	27,52,52	1.95	5 (18%)
4	ADP	G	2001	5	25,29,29	0.99	1 (4%)	25,45,45	1.82	3 (12%)
3	ATP	G	2004	5	27,33,33	0.97	1 (3%)	27,52,52	1.95	5 (18%)
4	ADP	H	2001	5	25,29,29	0.99	1 (4%)	25,45,45	1.83	3 (12%)
3	ATP	H	2004	5	27,33,33	0.98	1 (3%)	27,52,52	1.95	5 (18%)

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	501	-	-	0/18/38/38	0/3/3/3
3	ATP	A	502	-	-	0/18/38/38	0/3/3/3
3	ATP	C	501	-	-	0/18/38/38	0/3/3/3
3	ATP	D	501	-	-	0/18/38/38	0/3/3/3
4	ADP	E	2001	5	-	0/12/32/32	0/3/3/3
3	ATP	E	2004	5	-	0/18/38/38	0/3/3/3
4	ADP	F	2001	5	-	0/12/32/32	0/3/3/3
3	ATP	F	2004	5	-	0/18/38/38	0/3/3/3
4	ADP	G	2001	5	-	0/12/32/32	0/3/3/3
3	ATP	G	2004	5	-	0/18/38/38	0/3/3/3
4	ADP	H	2001	5	-	0/12/32/32	0/3/3/3
3	ATP	H	2004	5	-	0/18/38/38	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)
3	G	2004	ATP	C5-C4	2.90	1.47	1.40
3	E	2004	ATP	C5-C4	2.92	1.47	1.40
3	D	501	ATP	C5-C4	2.95	1.47	1.40
3	H	2004	ATP	C5-C4	2.95	1.47	1.40
4	G	2001	ADP	C5-C4	2.96	1.47	1.40

The worst 5 of 48 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	2001	ADP	N3-C2-N1	-6.27	123.49	128.86
4	E	2001	ADP	N3-C2-N1	-6.26	123.51	128.86
4	F	2001	ADP	N3-C2-N1	-6.23	123.53	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	G	2001	ADP	N3-C2-N1	-6.20	123.56	128.86
3	C	501	ATP	N3-C2-N1	-5.85	123.85	128.86

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

12 monomers are involved in 39 short contacts:

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

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.