



wwPDB EM Validation Summary Report ⓘ

Oct 14, 2024 – 12:48 PM JST

PDB ID : 5YWB
EMDB ID : EMD-6851
Title : Structure of pancreatic ATP-sensitive potassium channel bound with Mg-ADP
(CTD class2 at 5.2Å)
Authors : Chen, L.; Wu, J.X.
Deposited on : 2017-11-29
Resolution : 5.20 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ 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 ⓘ](#)) were used in the production of this report:

EMDB validation analysis : 0.0.1.dev113
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
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) : 2.39

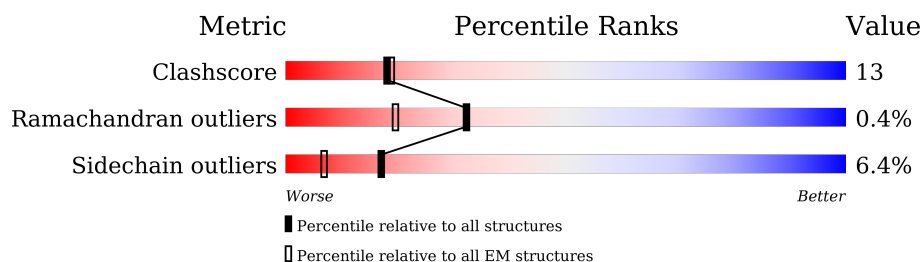
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 5.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	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 $\leq 5\%$. 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	390	<div> <div>7%</div> <div>54%</div> <div>26%</div> <div>•</div> <div>17%</div> </div>
1	C	390	<div> <div>7%</div> <div>53%</div> <div>26%</div> <div>•</div> <div>17%</div> </div>
1	E	390	<div> <div>7%</div> <div>54%</div> <div>25%</div> <div>•</div> <div>17%</div> </div>
1	G	390	<div> <div>7%</div> <div>53%</div> <div>26%</div> <div>•</div> <div>17%</div> </div>
2	B	1582	<div> <div>26%</div> <div>61%</div> <div>21%</div> <div>•</div> <div>16%</div> </div>
2	D	1582	<div> <div>26%</div> <div>61%</div> <div>21%</div> <div>•</div> <div>16%</div> </div>
2	F	1582	<div> <div>26%</div> <div>61%</div> <div>21%</div> <div>•</div> <div>16%</div> </div>
2	H	1582	<div> <div>26%</div> <div>61%</div> <div>21%</div> <div>•</div> <div>16%</div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 50928 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.

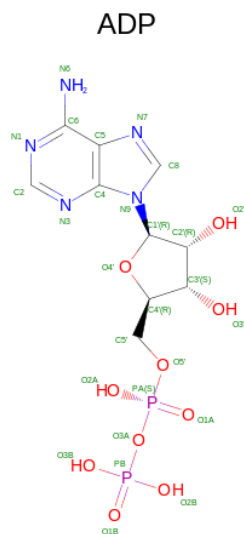
- Molecule 1 is a protein called ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	325	Total	C	N	O	S	0	0
			2424	1565	417	427	15		
1	C	325	Total	C	N	O	S	0	0
			2424	1565	417	427	15		
1	E	325	Total	C	N	O	S	0	0
			2424	1565	417	427	15		
1	G	325	Total	C	N	O	S	0	0
			2424	1565	417	427	15		

- Molecule 2 is a protein called ATP-binding cassette sub-family C member 8 isoform X2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1322	Total	C	N	O	S	0	0
			10225	6658	1727	1787	53		
2	D	1322	Total	C	N	O	S	0	0
			10225	6658	1727	1787	53		
2	F	1322	Total	C	N	O	S	0	0
			10225	6658	1727	1787	53		
2	H	1322	Total	C	N	O	S	0	0
			10225	6658	1727	1787	53		

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



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

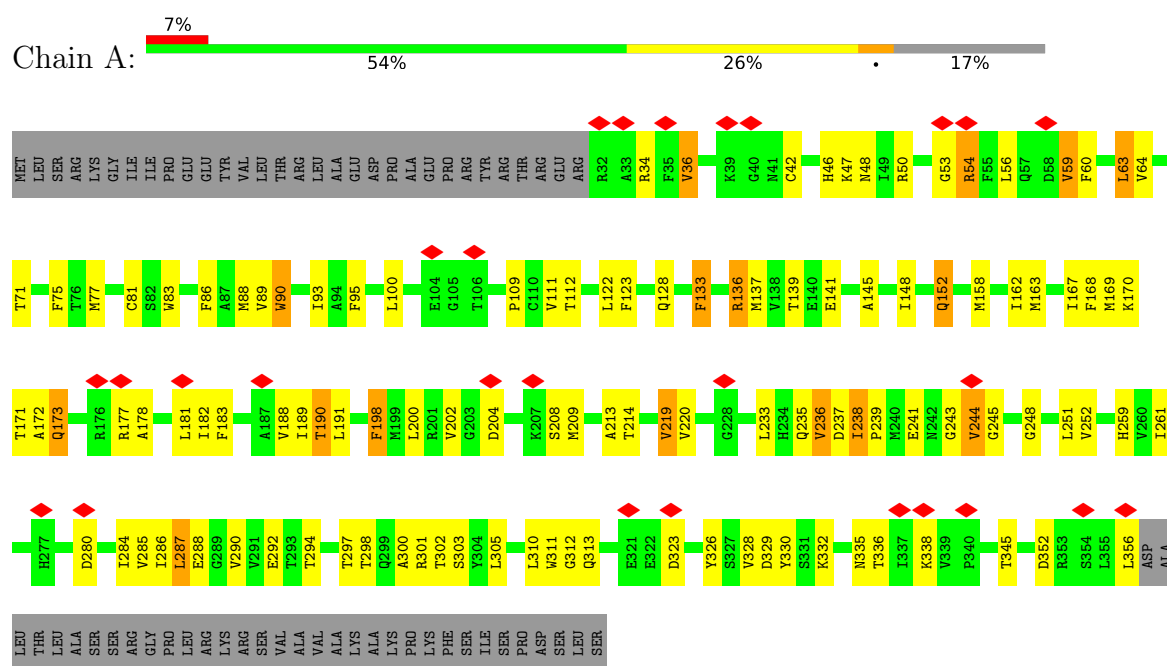
- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
4	B	2	Total 2	Mg 2	0
4	D	2	Total 2	Mg 2	0
4	F	2	Total 2	Mg 2	0
4	H	2	Total 2	Mg 2	0

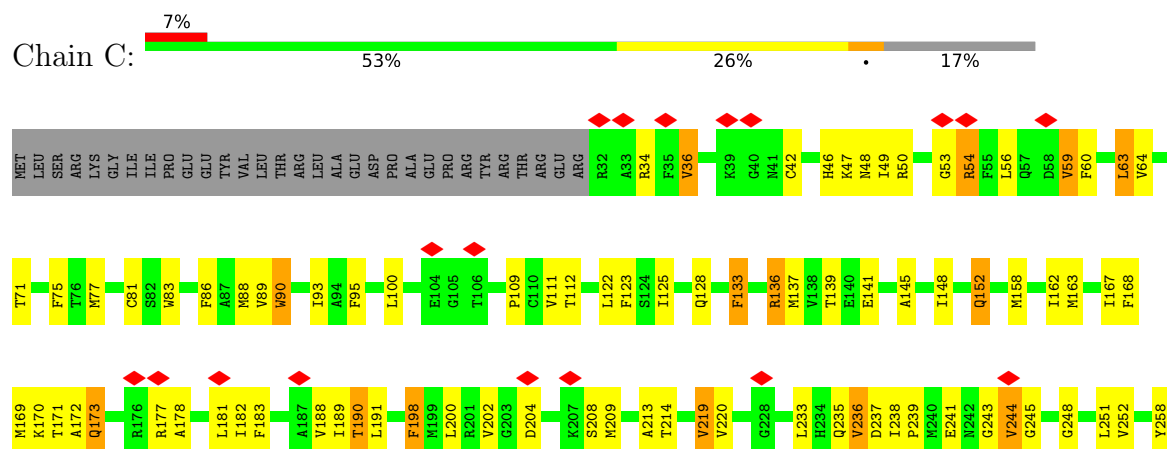
3 Residue-property plots [i](#)

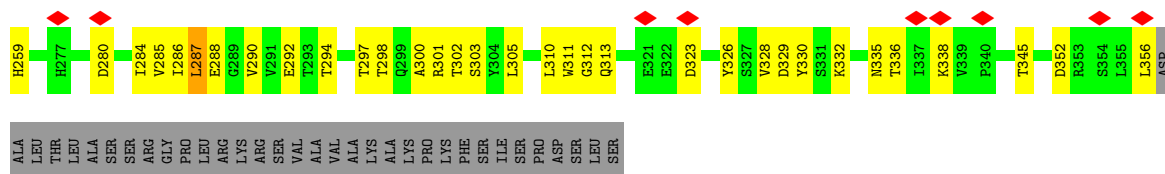
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

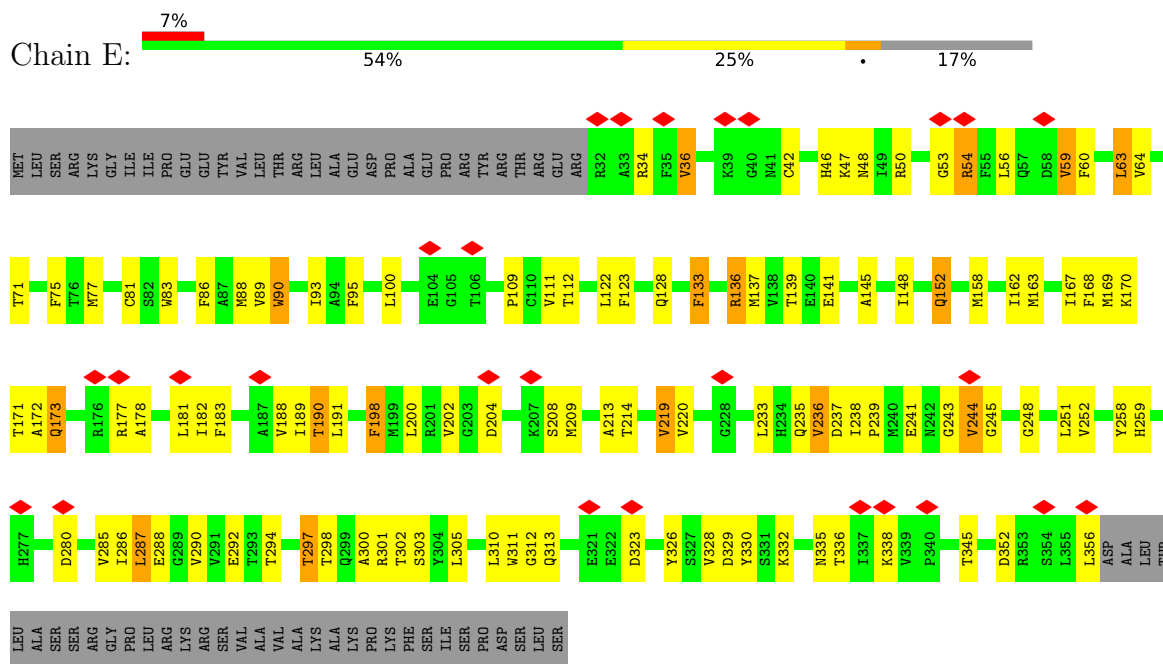


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

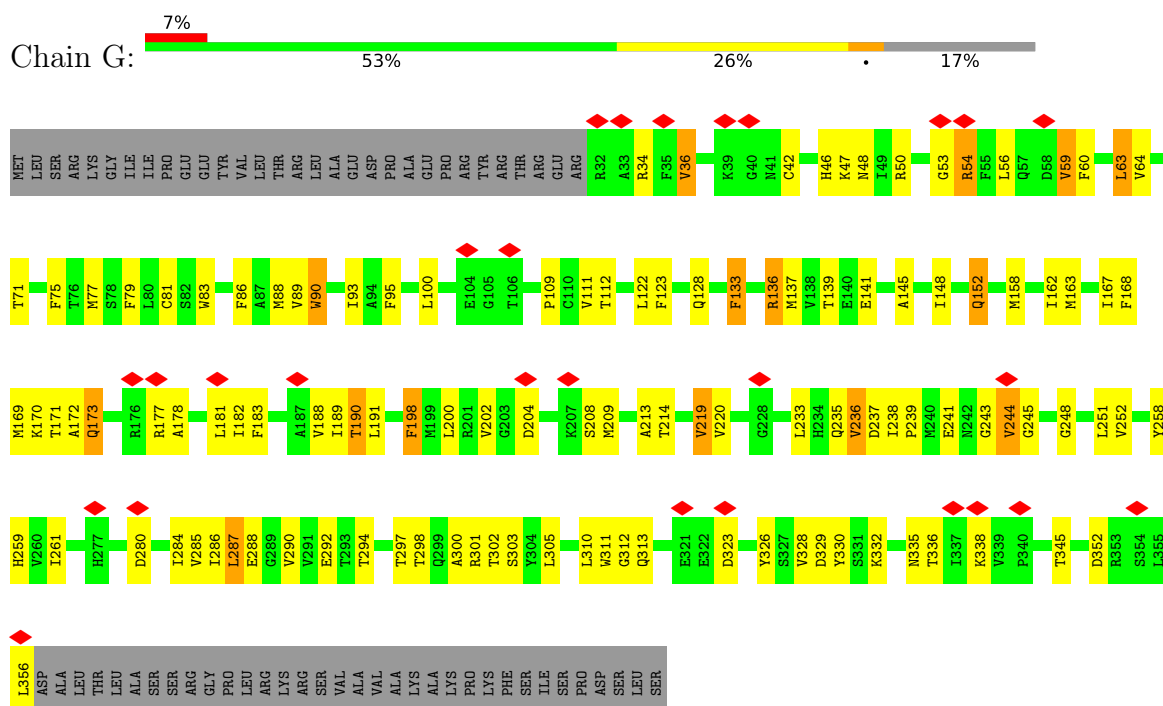




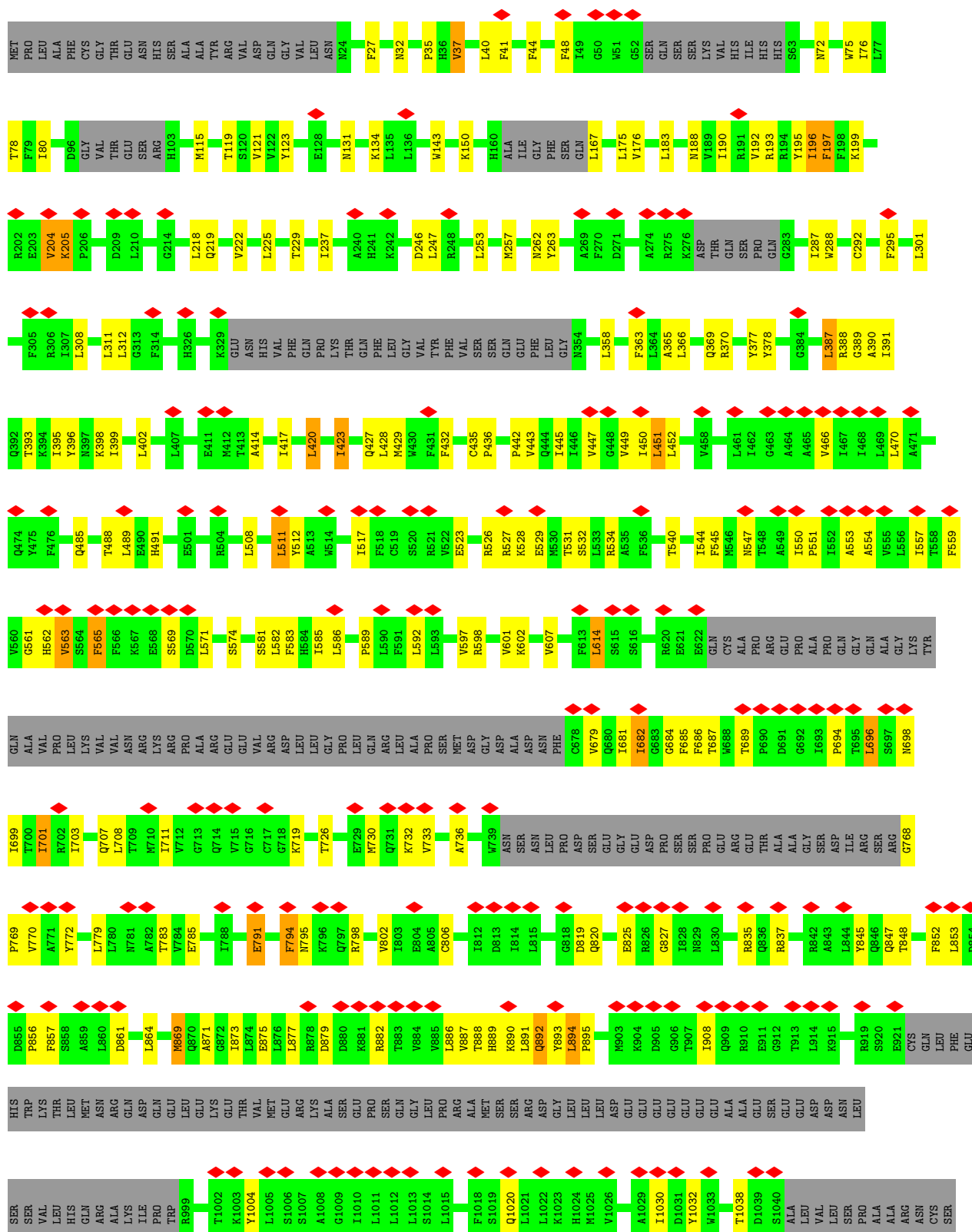
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

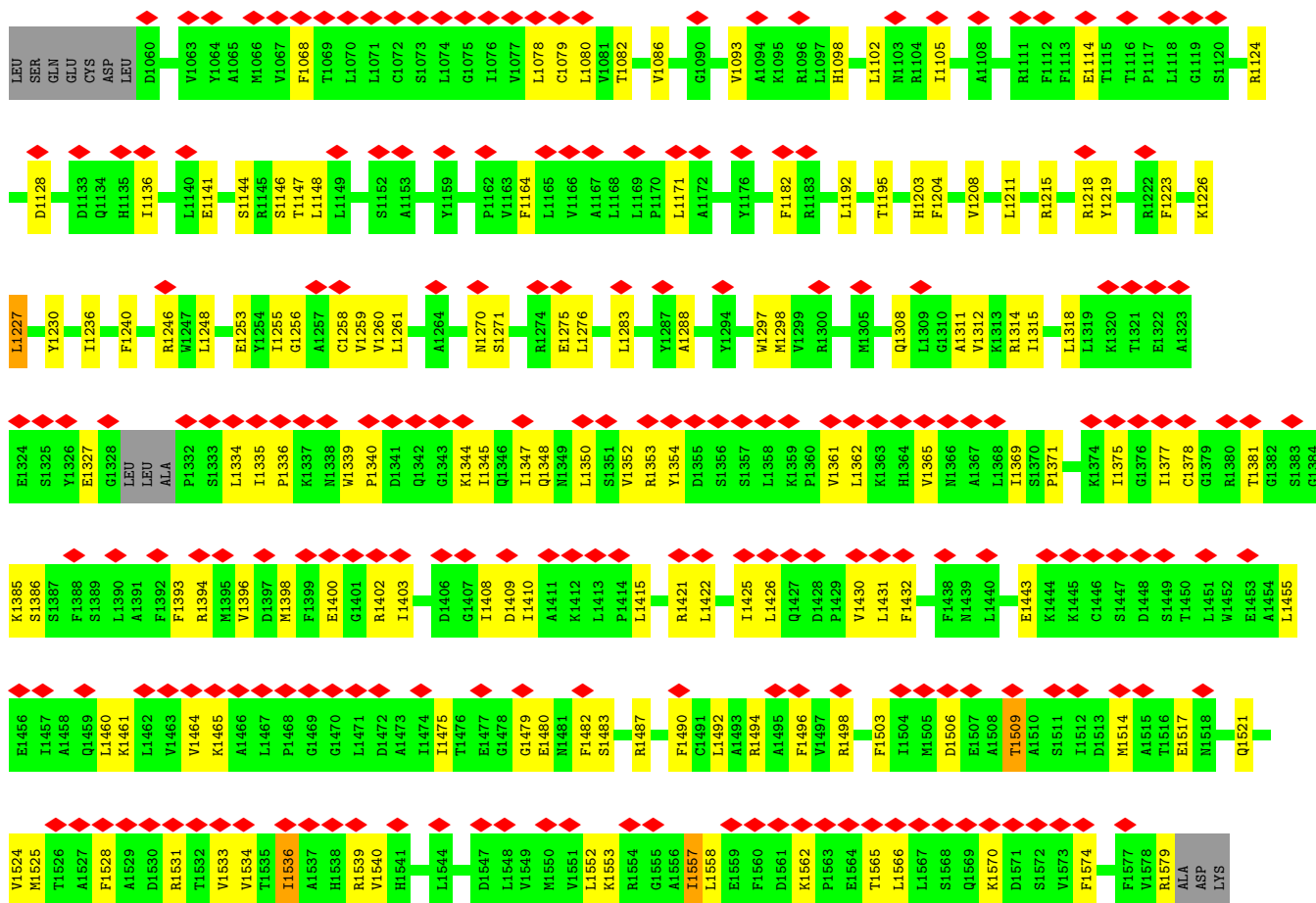


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

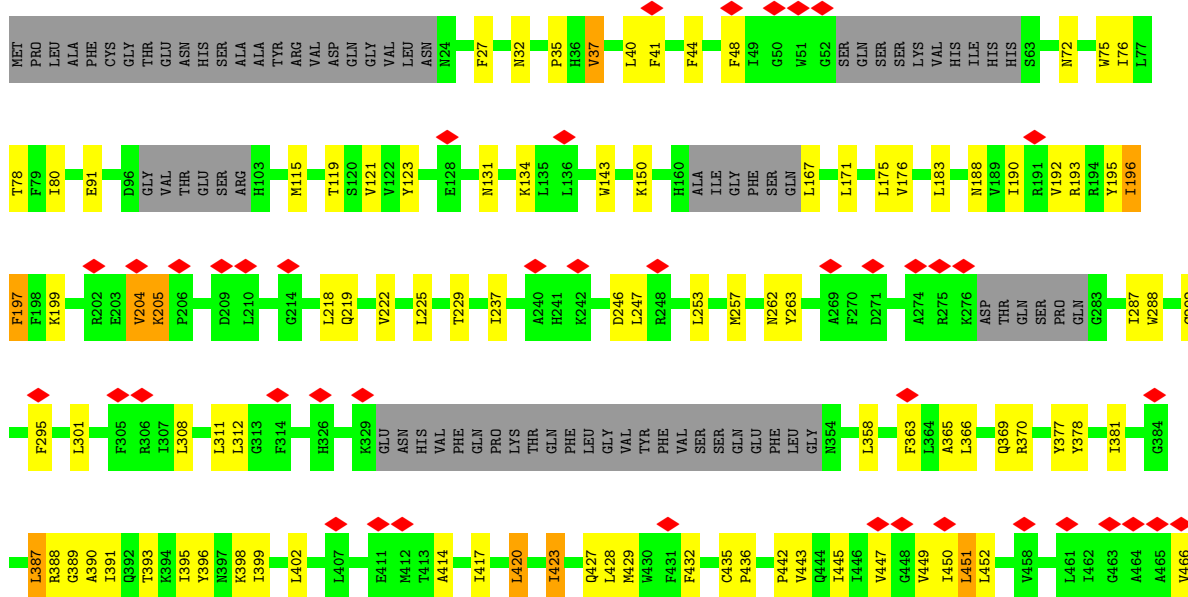


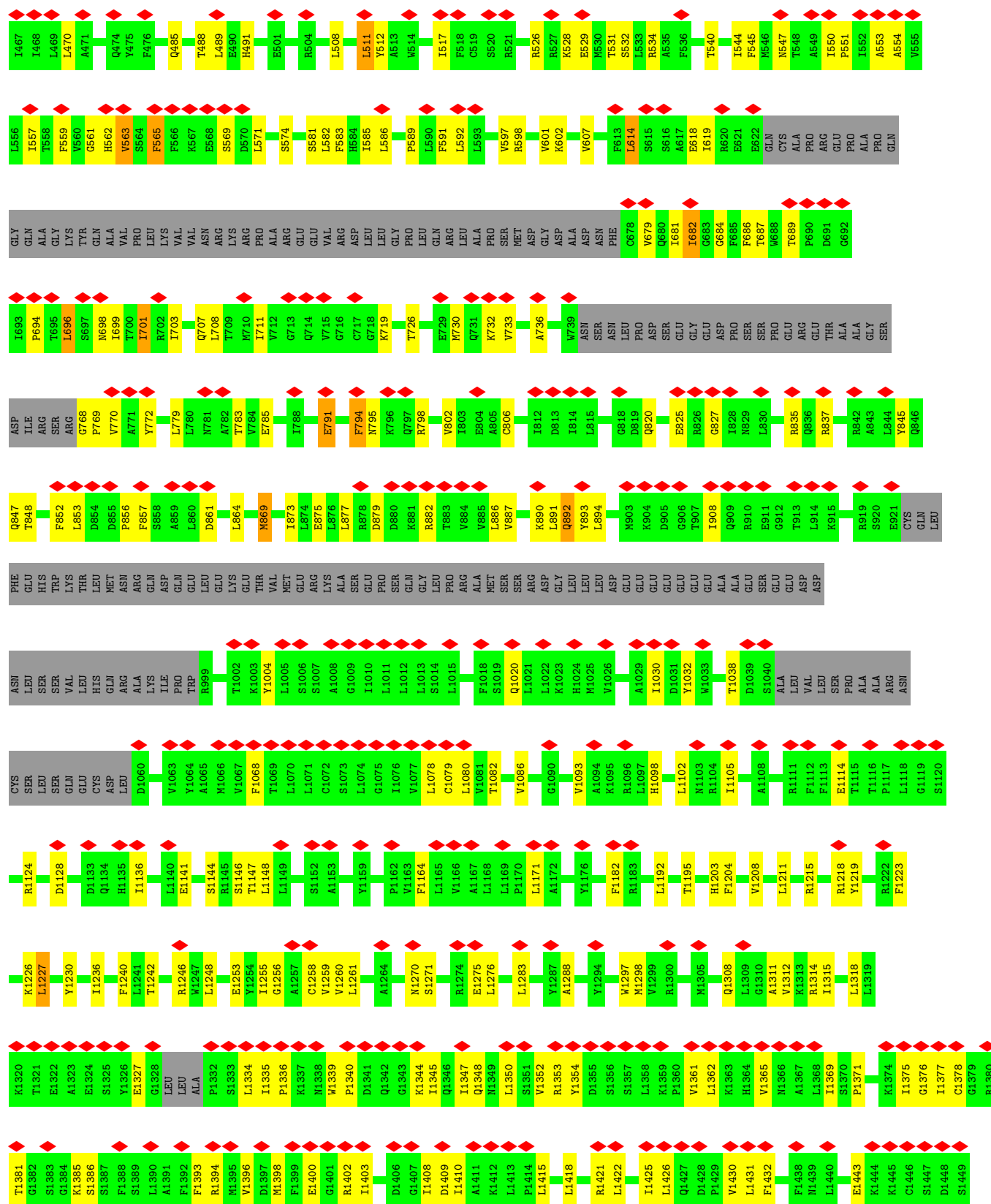
- Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

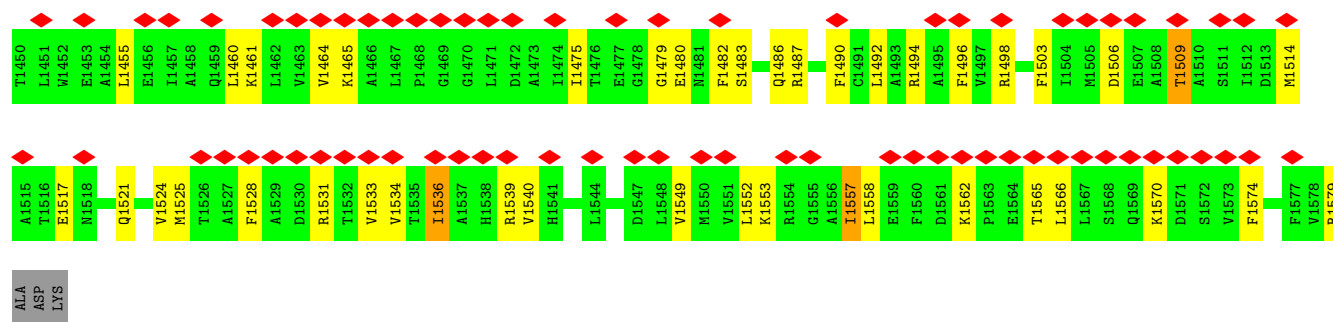




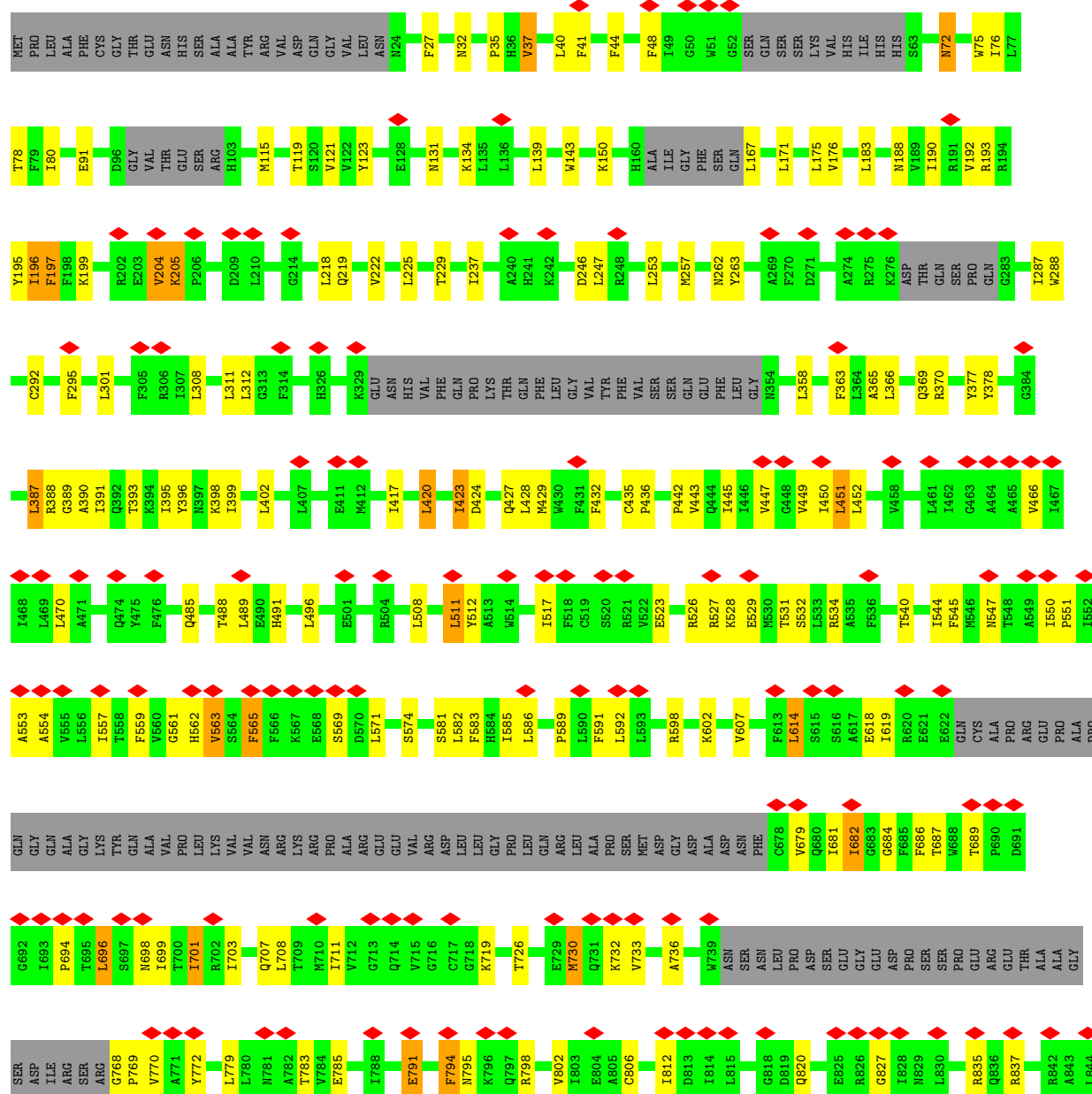
• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

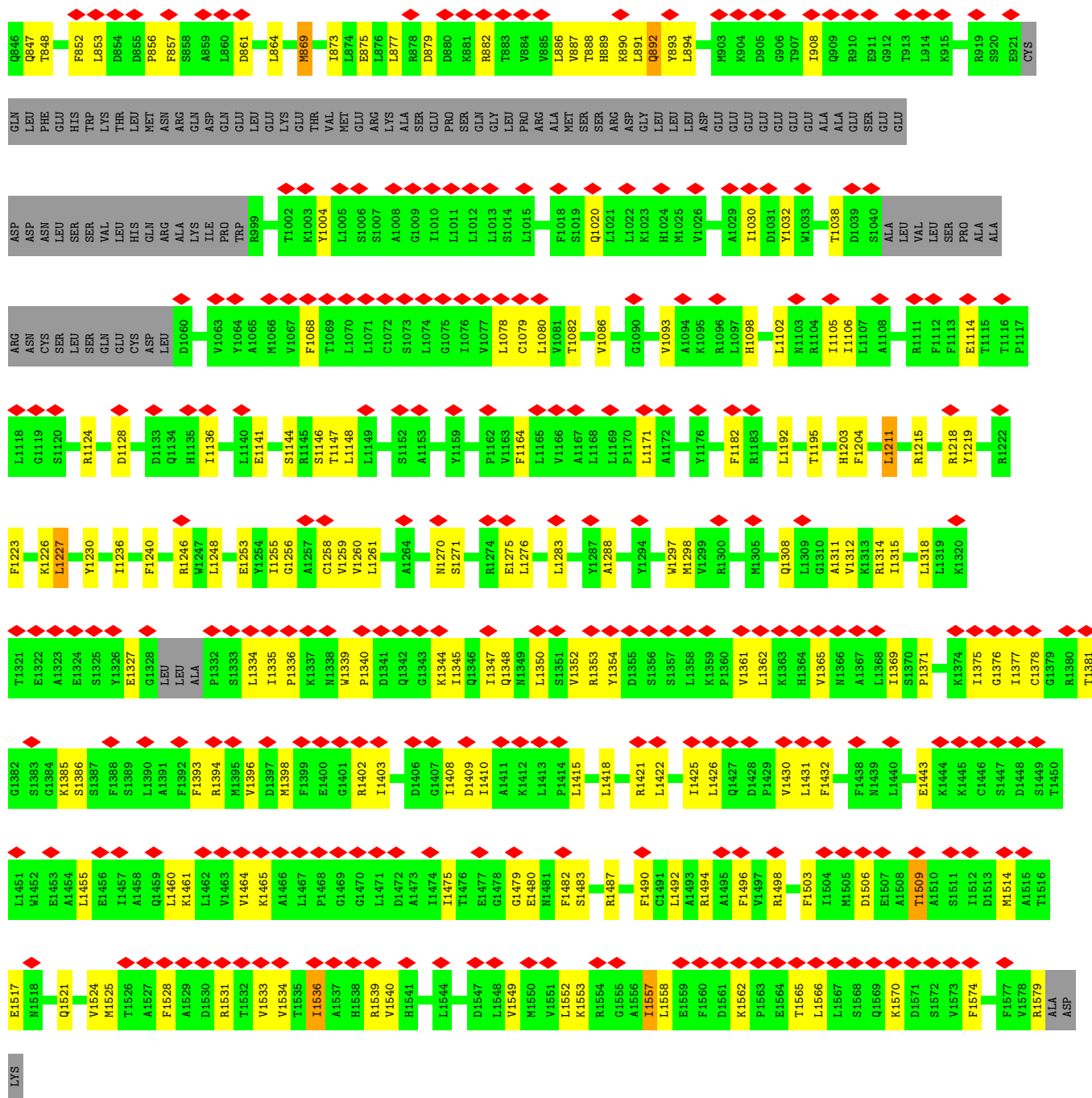




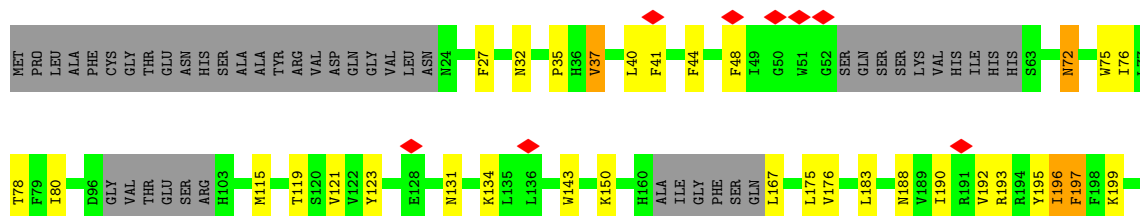


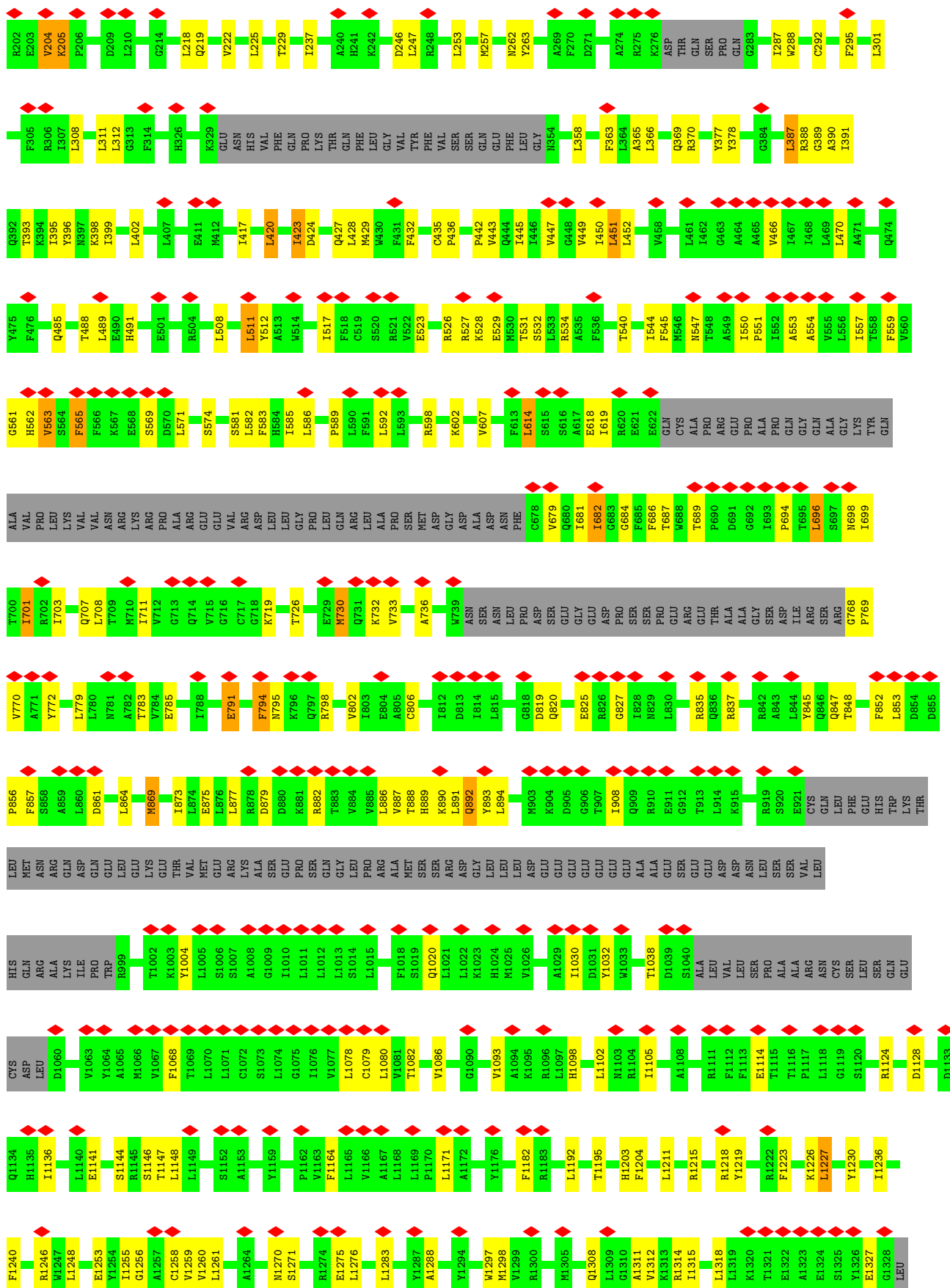
• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2





• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2





A1529	L1462	A1391	
D1530	V1463	F1392	
R1531	V1464	F1393	
T1532	K1465	R1394	
V1533	A1466	M1395	
V1534	L1467	V1396	
T1535	P1468	D1397	
I1536	G1469	M1398	
A1537	G1470	F1399	
H1538	L1471	E1400	
R1539	D1472	G1401	
V1540	A1473	R1402	
H1541	I1474	I1403	
	I1475	D1406	
L1544	T1476	G1407	
	E1477	I1408	
D1547	G1478	D1409	
L1548	G1479	I1410	
V1549	E1480	I1411	
M1550	N1481	K1412	
V1551	F1482	L1413	
K1552	S1483	P1414	
L1553		L1415	
R1554	Q1486		
G1555	R1487		
A1556			
I1557	F1490	R1421	
L1558	C1491	L1422	
E1559	L1492		
F1560	A1493	I1425	
D1561	R1494	L1426	
K1562	A1495	Q1427	
P1563	F1496	D1428	
E1564	V1497	P1429	
	R1498	V1430	
T1565	F1503	L1431	
L1566	I1504	F1432	
L1567	M1505		
S1568	D1506	F1438	
Q1569	E1507	M1439	
K1570	A1508	L1440	
D1571	T1509	E1443	
S1572	A1510	K1444	
V1573	S1511	K1445	
F1574	I1512	K1446	
	D1513	S1447	
	M1514	D1448	
F1577	A1515	L1449	
V1578	T1516	T1450	
R1579	E1517	L1451	
ALA	N1518	W1452	
ASP		R1380	
LYS	Q1521	T1381	
		E1453	
	V1524	L1454	
	M1525	E1456	
	T1526	I1457	
	A1527	A1458	
	F1528	Q1459	
		L1460	
		K1461	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56433	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.080	Depositor
Minimum map value	-0.030	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.025	Depositor
Map size (\AA)	329.15997, 329.15997, 329.15997	wwPDB
Map dimensions	312, 312, 312	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.055, 1.055, 1.055	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, ADP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.27	0/2477	0.48	0/3380
1	C	0.27	0/2477	0.48	0/3380
1	E	0.27	0/2477	0.48	0/3380
1	G	0.27	0/2477	0.48	0/3380
2	B	0.29	0/10430	0.46	0/14168
2	D	0.29	0/10430	0.46	0/14168
2	F	0.29	0/10430	0.46	0/14168
2	H	0.29	0/10430	0.46	0/14168
All	All	0.29	0/51628	0.47	0/70192

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2424	0	2383	105	0
1	C	2424	0	2383	105	0
1	E	2424	0	2383	104	0
1	G	2424	0	2383	105	0
2	B	10225	0	10456	245	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	10225	0	10456	248	0
2	F	10225	0	10456	250	0
2	H	10225	0	10456	242	0
3	A	27	0	12	0	0
3	B	54	0	24	4	0
3	C	27	0	12	0	0
3	D	54	0	24	3	0
3	E	27	0	12	0	0
3	F	54	0	24	3	0
3	G	27	0	12	0	0
3	H	54	0	24	4	0
4	B	2	0	0	0	0
4	D	2	0	0	0	0
4	F	2	0	0	0	0
4	H	2	0	0	0	0
All	All	50928	0	51500	1335	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 13.

The worst 5 of 1335 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:D:190:ILE:HG13	2:D:195:TYR:CB	1.79	1.13
2:F:190:ILE:HG13	2:F:195:TYR:CB	1.79	1.13
2:H:190:ILE:HG13	2:H:195:TYR:CB	1.79	1.12
2:B:190:ILE:HG13	2:B:195:TYR:CB	1.79	1.11
1:A:172:ALA:HA	1:G:169:MET:HE1	1.34	1.05

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	323/390 (83%)	305 (94%)	15 (5%)	3 (1%)	14	50
1	C	323/390 (83%)	305 (94%)	15 (5%)	3 (1%)	14	50
1	E	323/390 (83%)	305 (94%)	15 (5%)	3 (1%)	14	50
1	G	323/390 (83%)	305 (94%)	15 (5%)	3 (1%)	14	50
2	B	1300/1582 (82%)	1245 (96%)	51 (4%)	4 (0%)	37	72
2	D	1300/1582 (82%)	1245 (96%)	51 (4%)	4 (0%)	37	72
2	F	1300/1582 (82%)	1245 (96%)	51 (4%)	4 (0%)	37	72
2	H	1300/1582 (82%)	1245 (96%)	51 (4%)	4 (0%)	37	72
All	All	6492/7888 (82%)	6200 (96%)	264 (4%)	28 (0%)	32	68

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	50	ARG
1	A	54	ARG
2	B	197	PHE
2	B	199	LYS
1	C	50	ARG

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	250/339 (74%)	223 (89%)	27 (11%)	5	19
1	C	250/339 (74%)	223 (89%)	27 (11%)	5	19
1	E	250/339 (74%)	223 (89%)	27 (11%)	5	19
1	G	250/339 (74%)	223 (89%)	27 (11%)	5	19
2	B	1095/1371 (80%)	1036 (95%)	59 (5%)	18	40
2	D	1095/1371 (80%)	1036 (95%)	59 (5%)	18	40
2	F	1095/1371 (80%)	1036 (95%)	59 (5%)	18	40
2	H	1095/1371 (80%)	1036 (95%)	59 (5%)	18	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	5380/6840 (79%)	5036 (94%)	344 (6%)	17	36

5 of 344 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	708	LEU
2	H	72	ASN
2	F	891	LEU
1	G	63	LEU
2	H	420	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 30 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	474	GLN
1	G	259	HIS
1	E	128	GLN
2	H	1203	HIS
1	G	128	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 oligosaccharides 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	ADP	C	401	-	24,29,29	0.99	1 (4%)	29,45,45	1.45	4 (13%)
3	ADP	D	2502	4	24,29,29	0.93	1 (4%)	29,45,45	1.33	4 (13%)
3	ADP	B	2502	4	24,29,29	0.93	1 (4%)	29,45,45	1.33	4 (13%)
3	ADP	E	401	-	24,29,29	0.99	1 (4%)	29,45,45	1.45	4 (13%)
3	ADP	H	2502	4	24,29,29	0.93	1 (4%)	29,45,45	1.33	4 (13%)
3	ADP	G	401	-	24,29,29	0.99	1 (4%)	29,45,45	1.45	4 (13%)
3	ADP	F	2502	4	24,29,29	0.93	1 (4%)	29,45,45	1.33	4 (13%)
3	ADP	H	2501	4	24,29,29	0.92	1 (4%)	29,45,45	1.37	4 (13%)
3	ADP	D	2501	4	24,29,29	0.92	1 (4%)	29,45,45	1.37	4 (13%)
3	ADP	F	2501	4	24,29,29	0.92	1 (4%)	29,45,45	1.37	4 (13%)
3	ADP	A	401	-	24,29,29	0.99	1 (4%)	29,45,45	1.45	4 (13%)
3	ADP	B	2501	4	24,29,29	0.92	1 (4%)	29,45,45	1.37	4 (13%)

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	C	401	-	-	4/12/32/32	0/3/3/3
3	ADP	D	2502	4	-	4/12/32/32	0/3/3/3
3	ADP	B	2502	4	-	4/12/32/32	0/3/3/3
3	ADP	E	401	-	-	4/12/32/32	0/3/3/3
3	ADP	H	2502	4	-	4/12/32/32	0/3/3/3
3	ADP	G	401	-	-	4/12/32/32	0/3/3/3
3	ADP	F	2502	4	-	4/12/32/32	0/3/3/3
3	ADP	H	2501	4	-	2/12/32/32	0/3/3/3
3	ADP	D	2501	4	-	2/12/32/32	0/3/3/3
3	ADP	F	2501	4	-	2/12/32/32	0/3/3/3
3	ADP	A	401	-	-	4/12/32/32	0/3/3/3
3	ADP	B	2501	4	-	2/12/32/32	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	A	401	ADP	C5-C4	2.46	1.47	1.40
3	C	401	ADP	C5-C4	2.46	1.47	1.40
3	E	401	ADP	C5-C4	2.46	1.47	1.40
3	G	401	ADP	C5-C4	2.46	1.47	1.40
3	B	2502	ADP	C5-C4	2.44	1.47	1.40

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	401	ADP	PA-O3A-PB	-4.01	119.06	132.83
3	C	401	ADP	PA-O3A-PB	-4.01	119.06	132.83
3	E	401	ADP	PA-O3A-PB	-4.01	119.06	132.83
3	G	401	ADP	PA-O3A-PB	-4.01	119.06	132.83
3	A	401	ADP	C3'-C2'-C1'	3.40	106.09	100.98

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	401	ADP	O4'-C4'-C5'-O5'
3	B	2502	ADP	C5'-O5'-PA-O3A
3	B	2502	ADP	O4'-C4'-C5'-O5'
3	B	2502	ADP	C3'-C4'-C5'-O5'
3	C	401	ADP	O4'-C4'-C5'-O5'

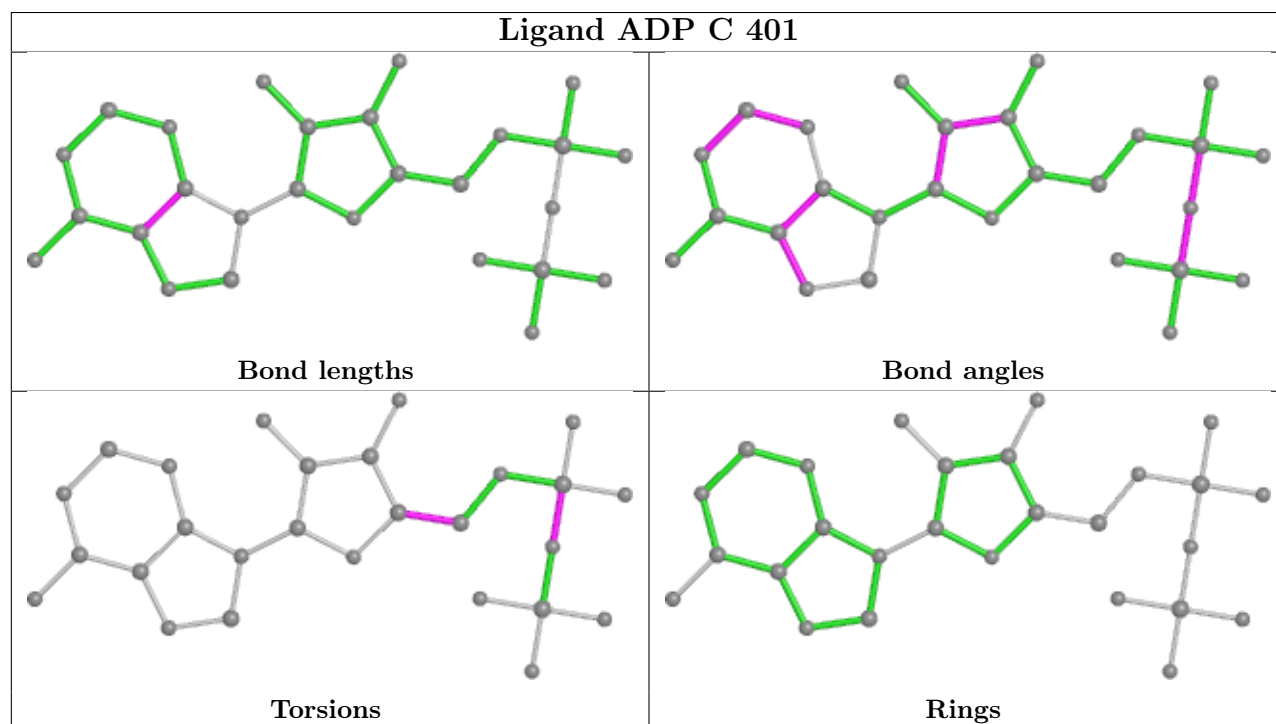
There are no ring outliers.

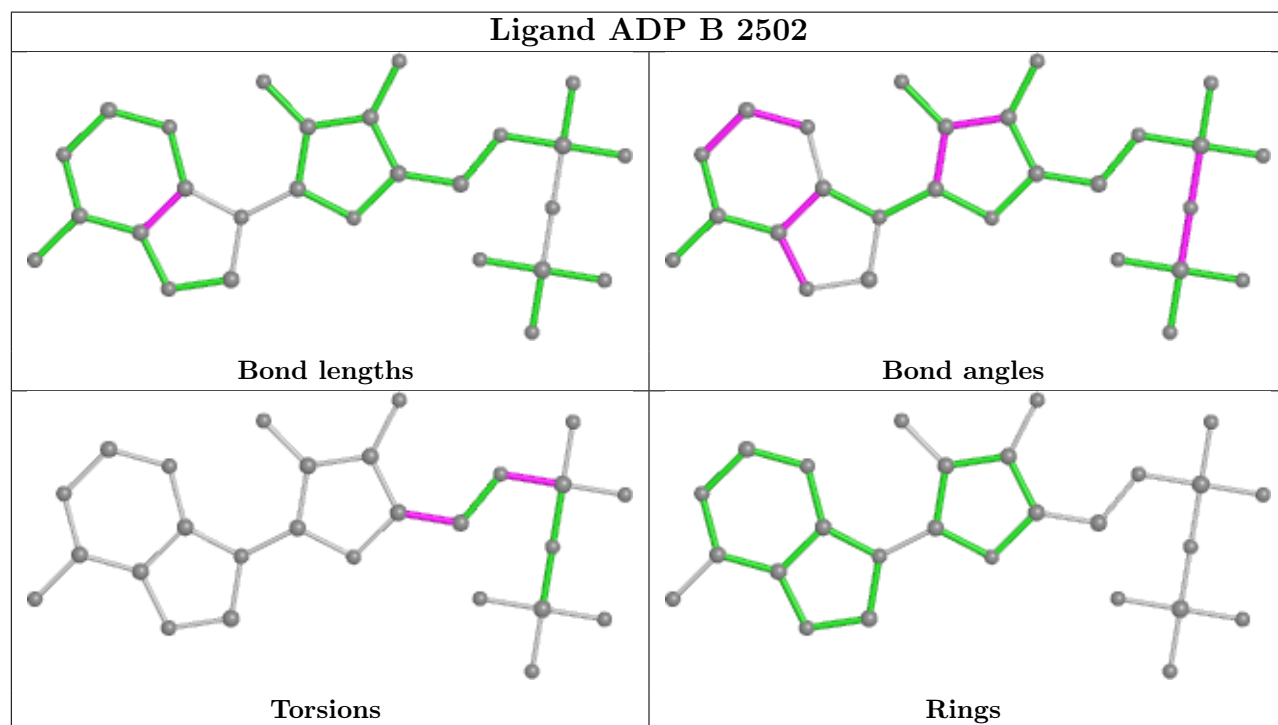
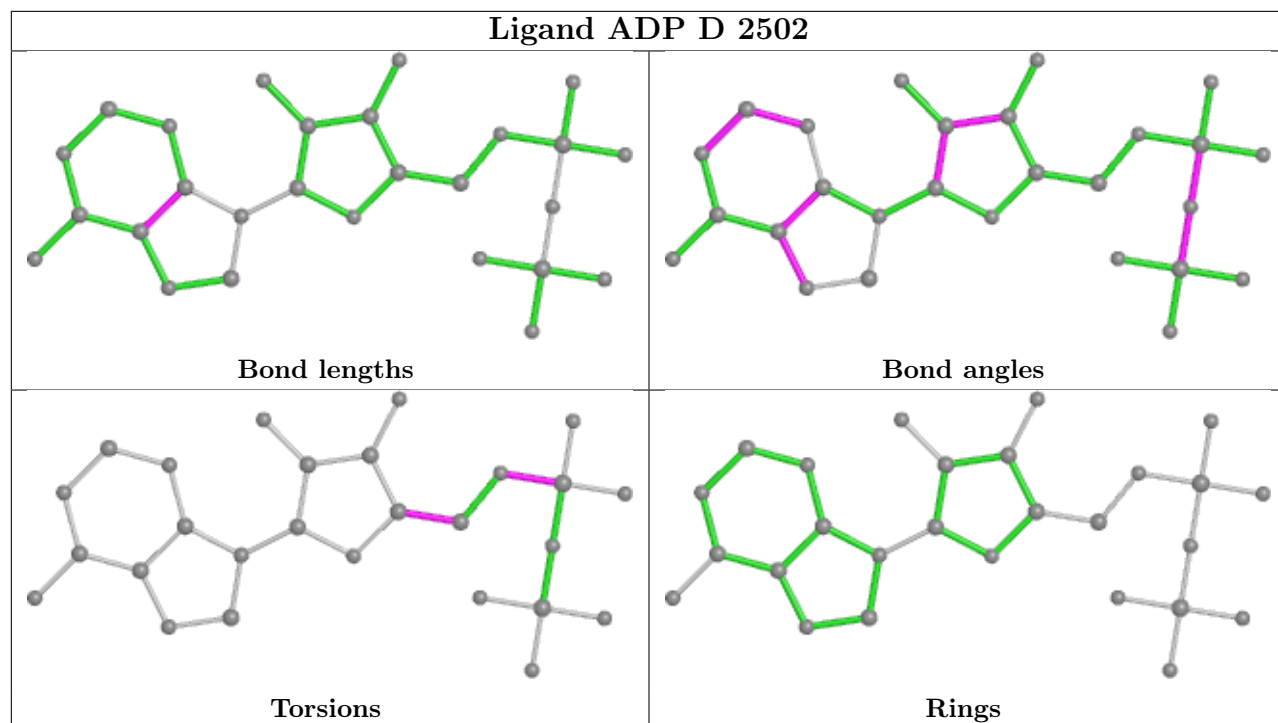
8 monomers are involved in 14 short contacts:

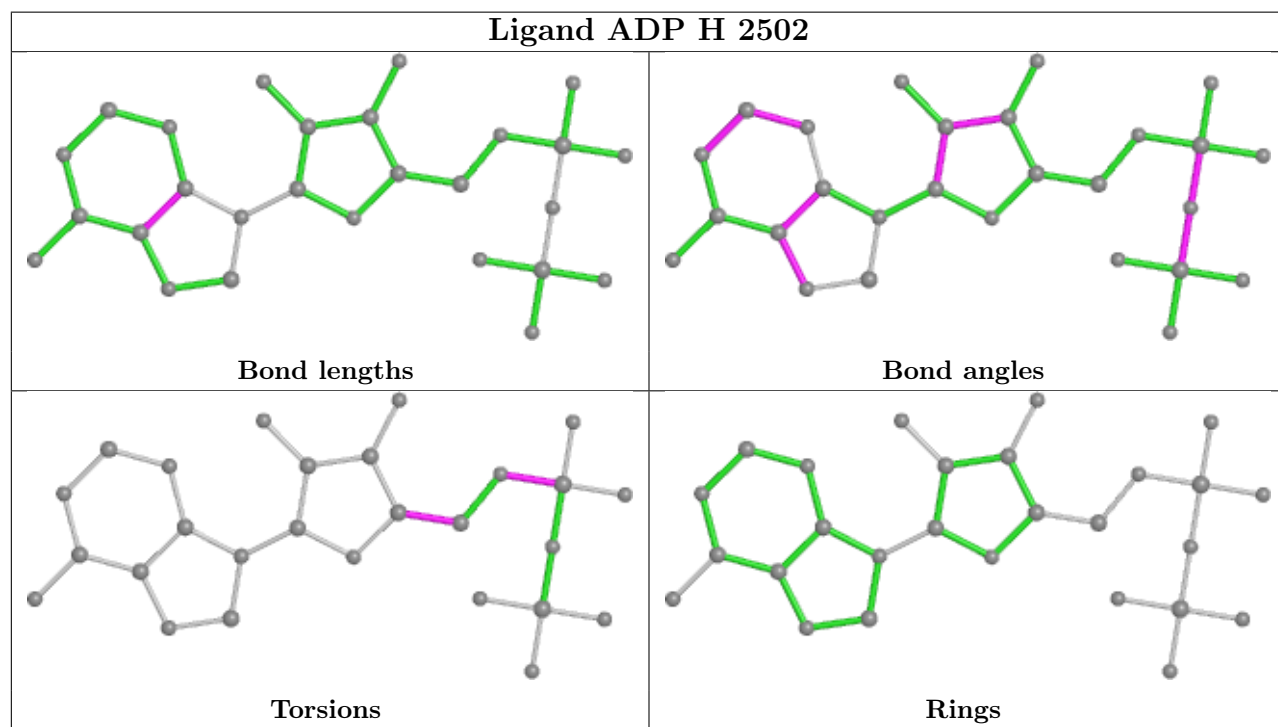
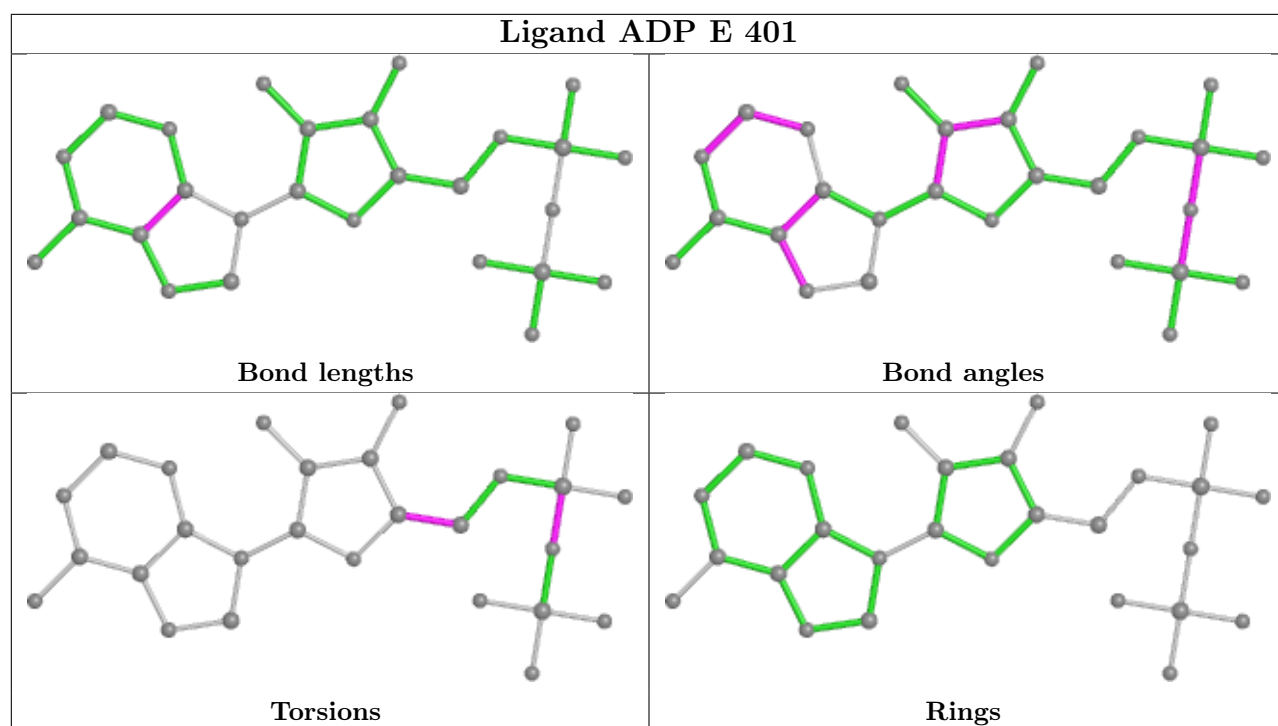
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	2502	ADP	2	0
3	B	2502	ADP	2	0
3	H	2502	ADP	2	0
3	F	2502	ADP	2	0
3	H	2501	ADP	2	0
3	D	2501	ADP	1	0
3	F	2501	ADP	1	0
3	B	2501	ADP	2	0

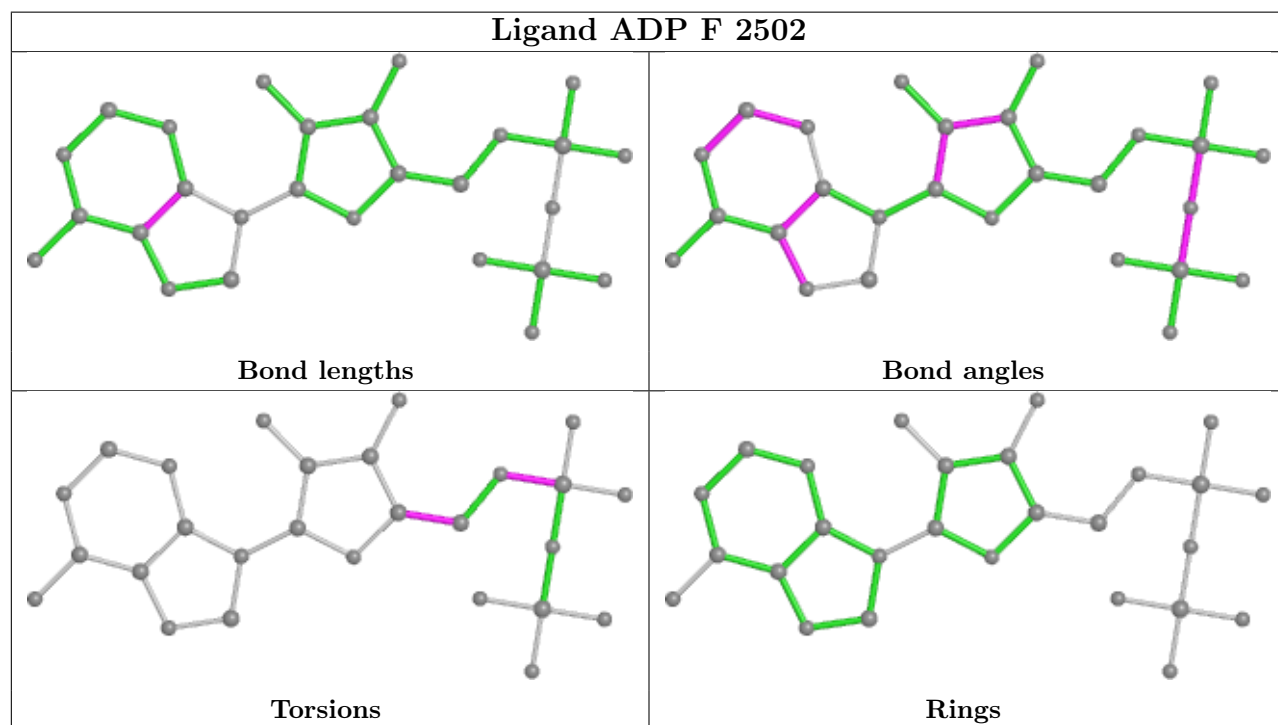
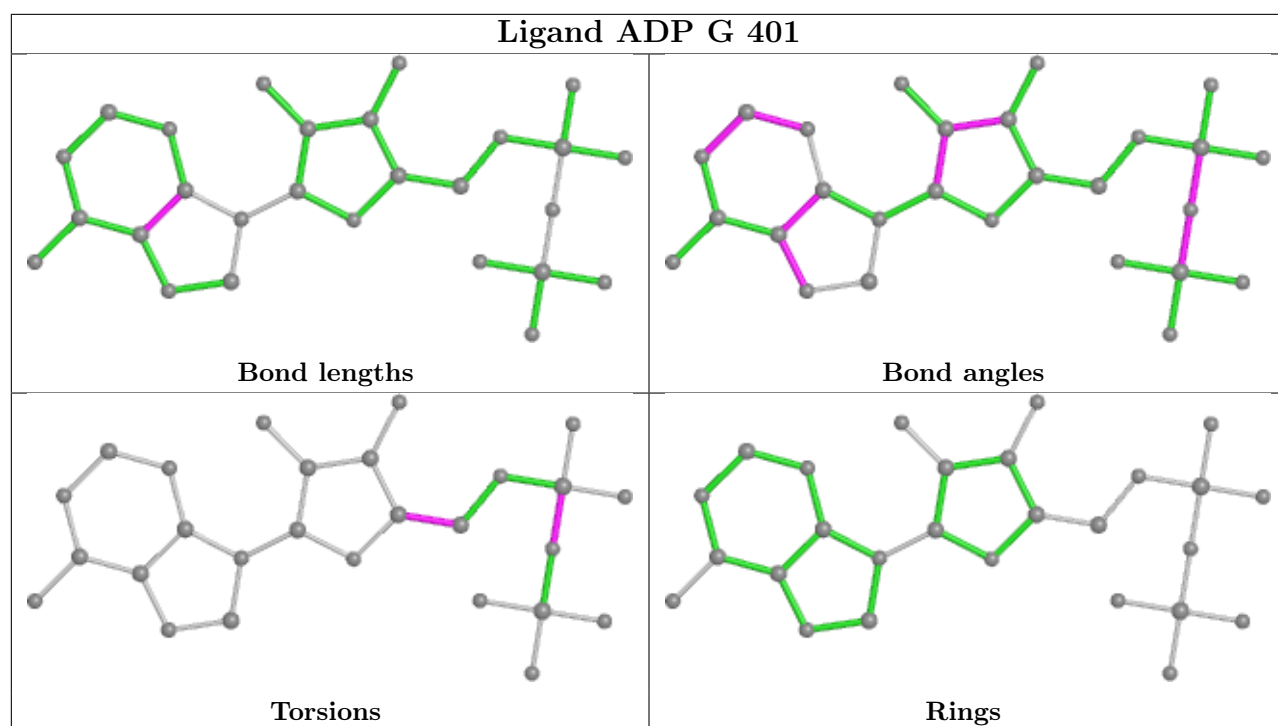
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

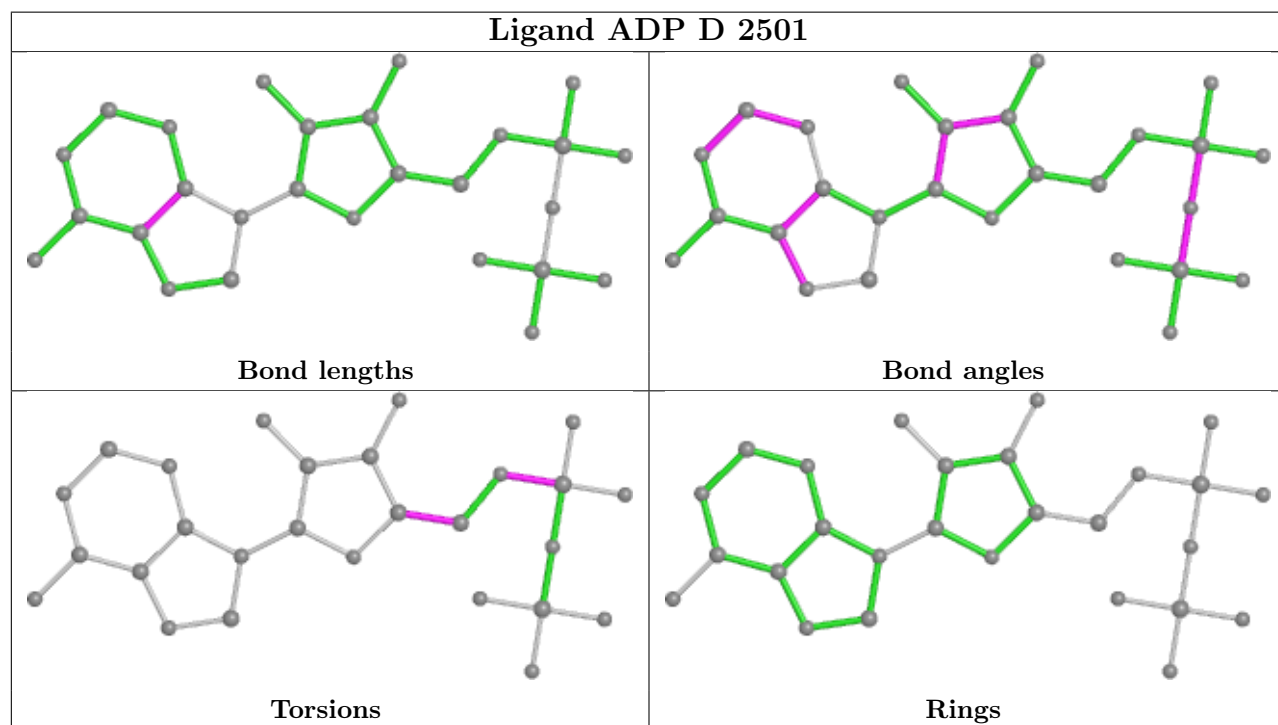
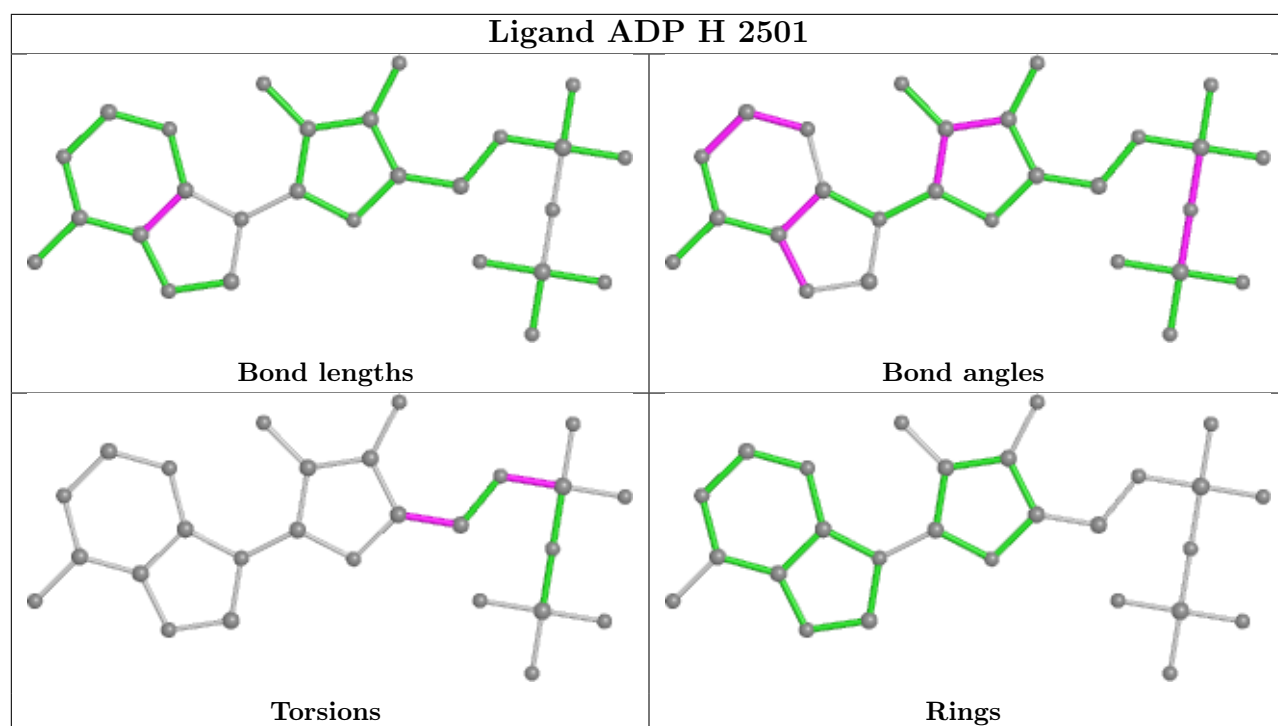
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted 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.

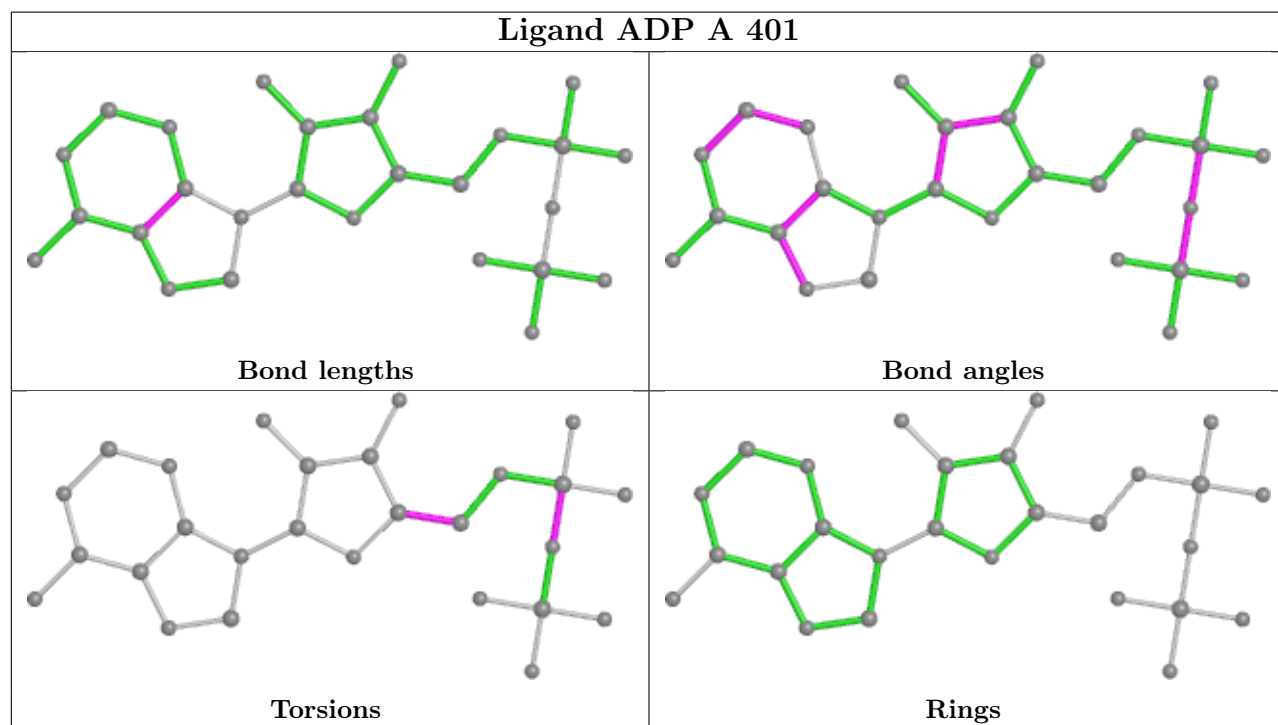
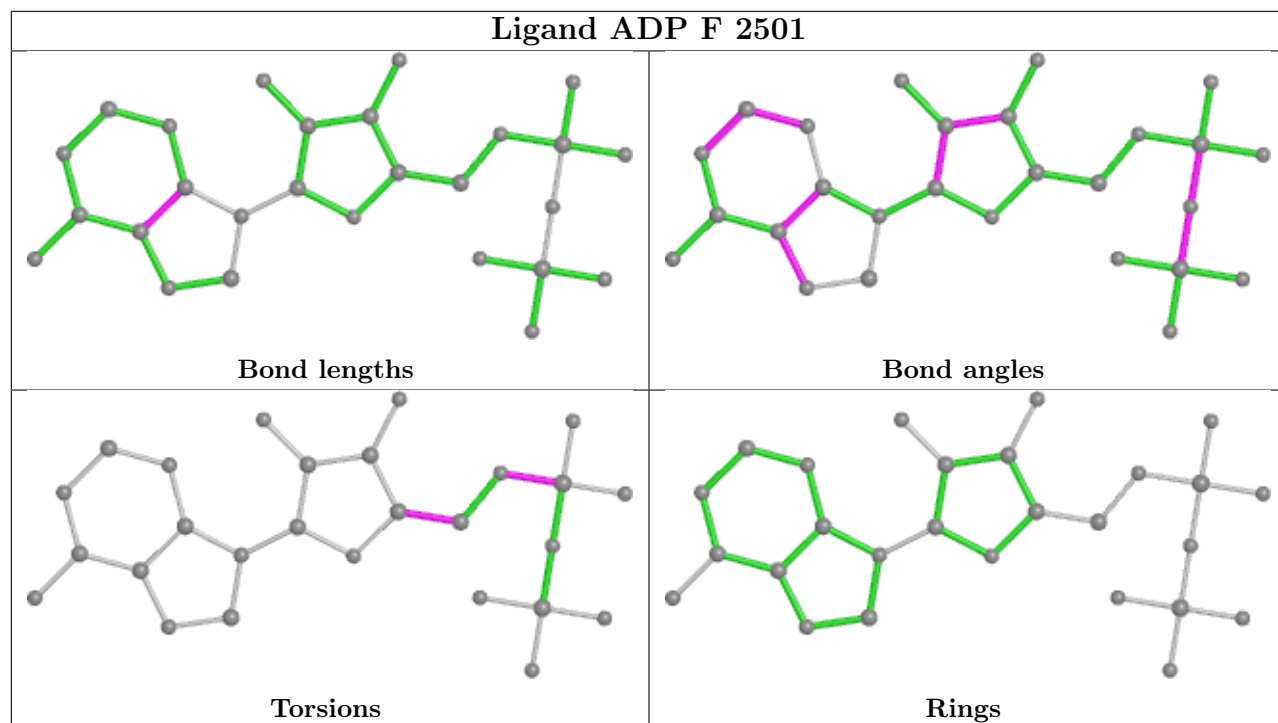


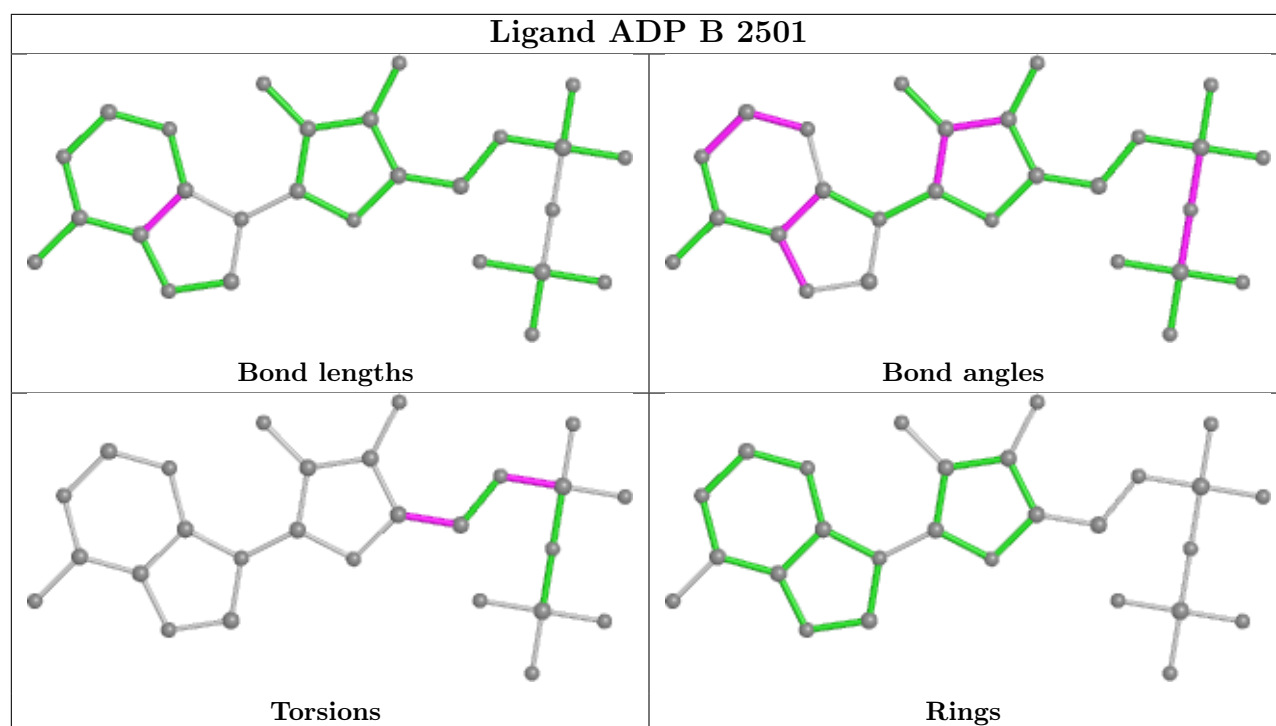












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

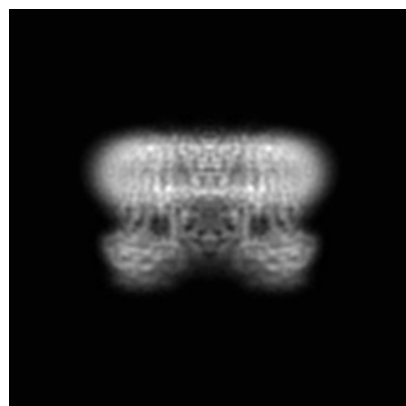
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6851. These allow visual inspection of the internal detail of the map and identification of artifacts.

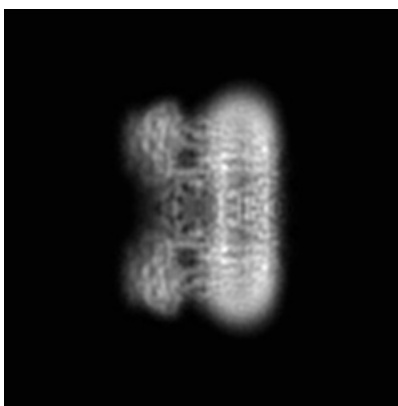
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

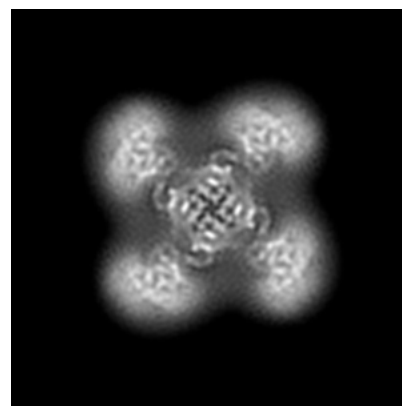
6.1.1 Primary map



X

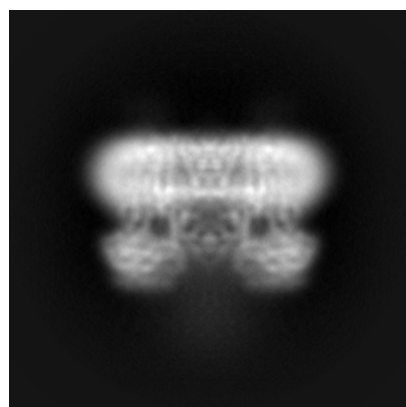


Y

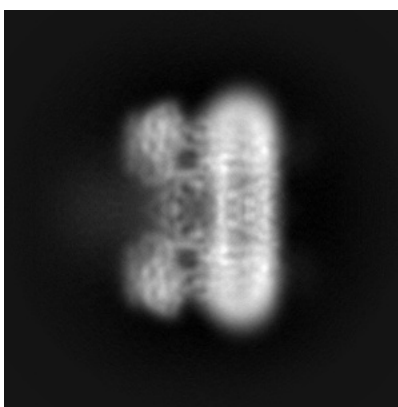


Z

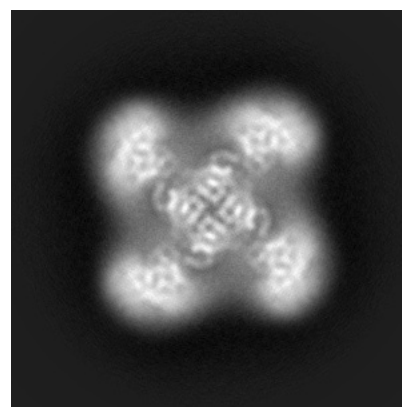
6.1.2 Raw map



X



Y



Z

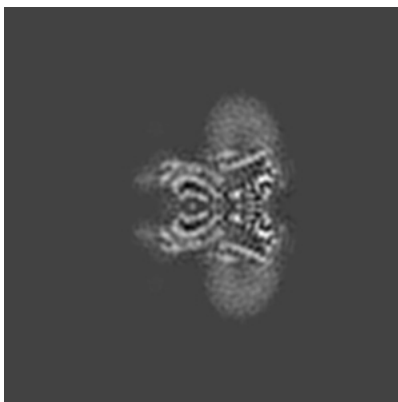
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

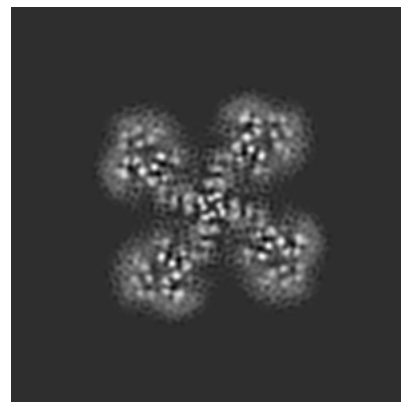
6.2.1 Primary map



X Index: 156

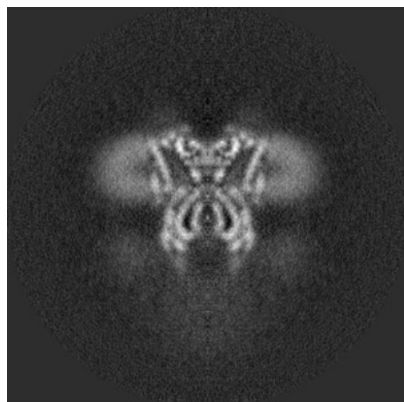


Y Index: 156

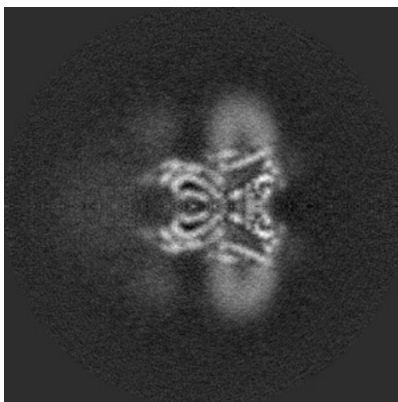


Z Index: 156

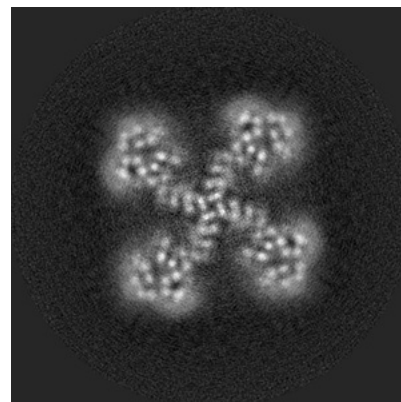
6.2.2 Raw map



X Index: 156



Y Index: 156



Z Index: 156

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

6.3 Largest variance slices [i](#)

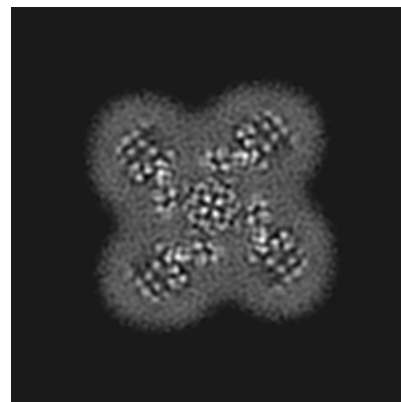
6.3.1 Primary map



X Index: 196

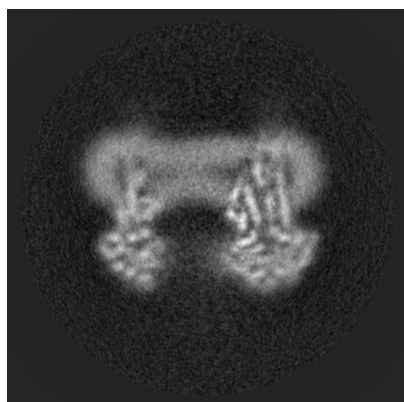


Y Index: 116

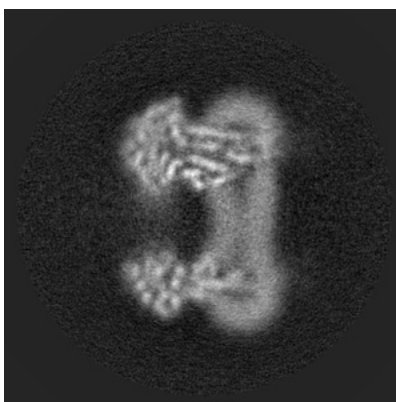


Z Index: 170

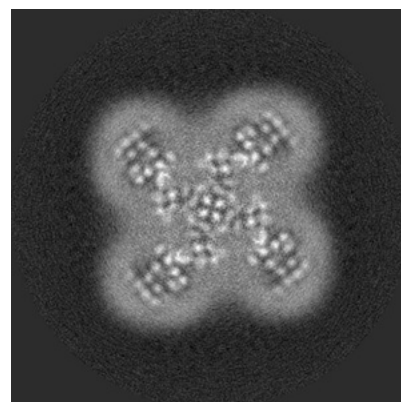
6.3.2 Raw map



X Index: 98



Y Index: 214

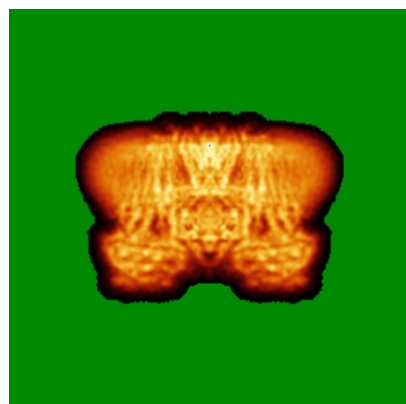


Z Index: 170

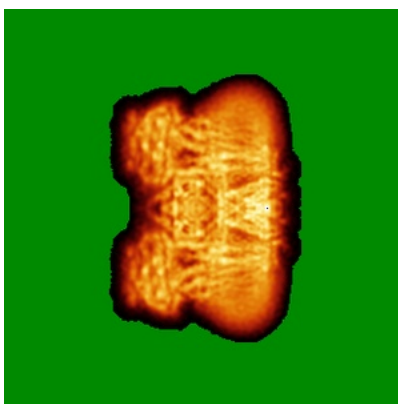
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

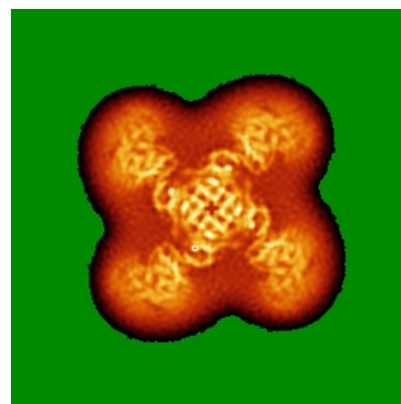
6.4.1 Primary map



X

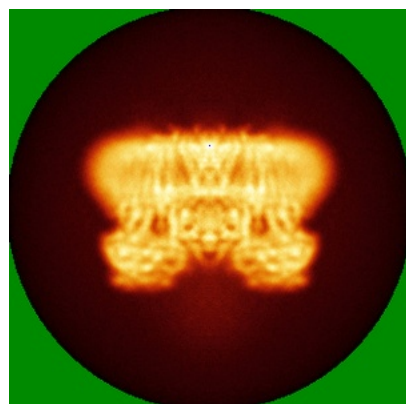


Y

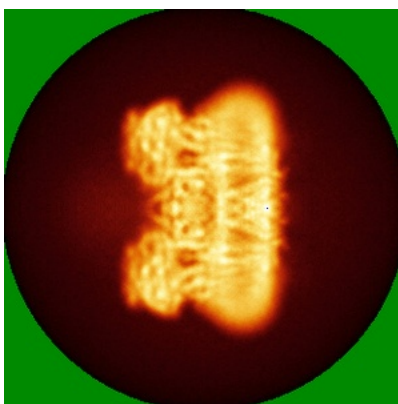


Z

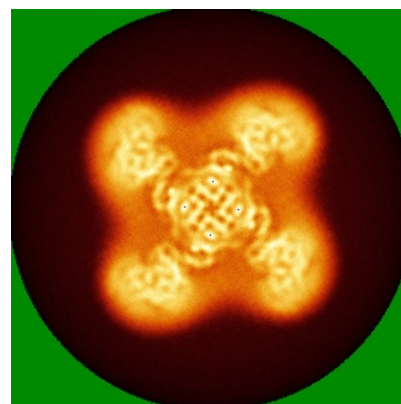
6.4.2 Raw map



X



Y

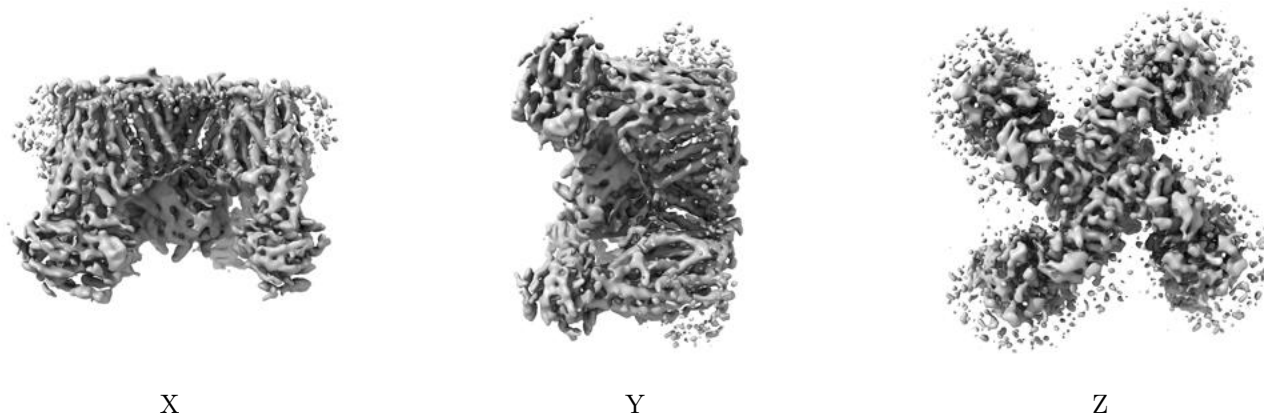


Z

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.

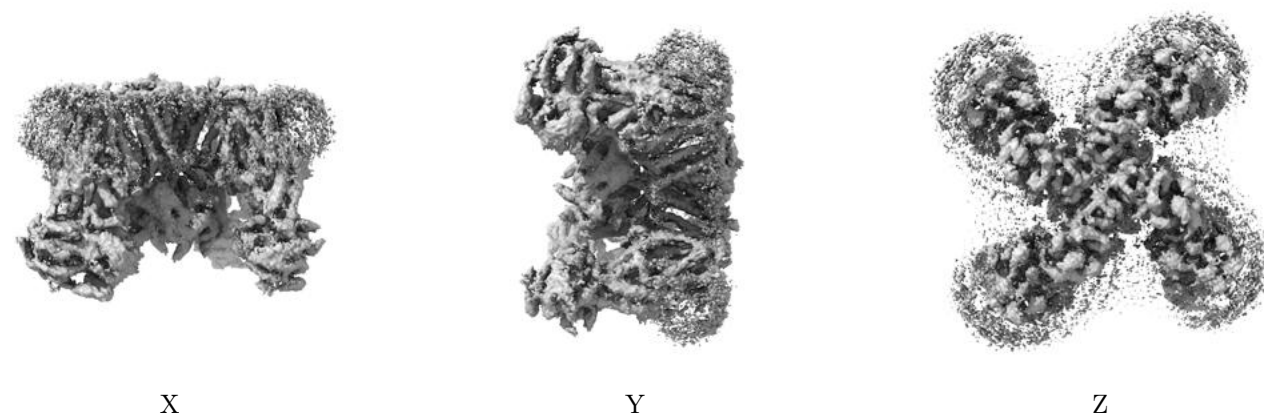
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.025. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

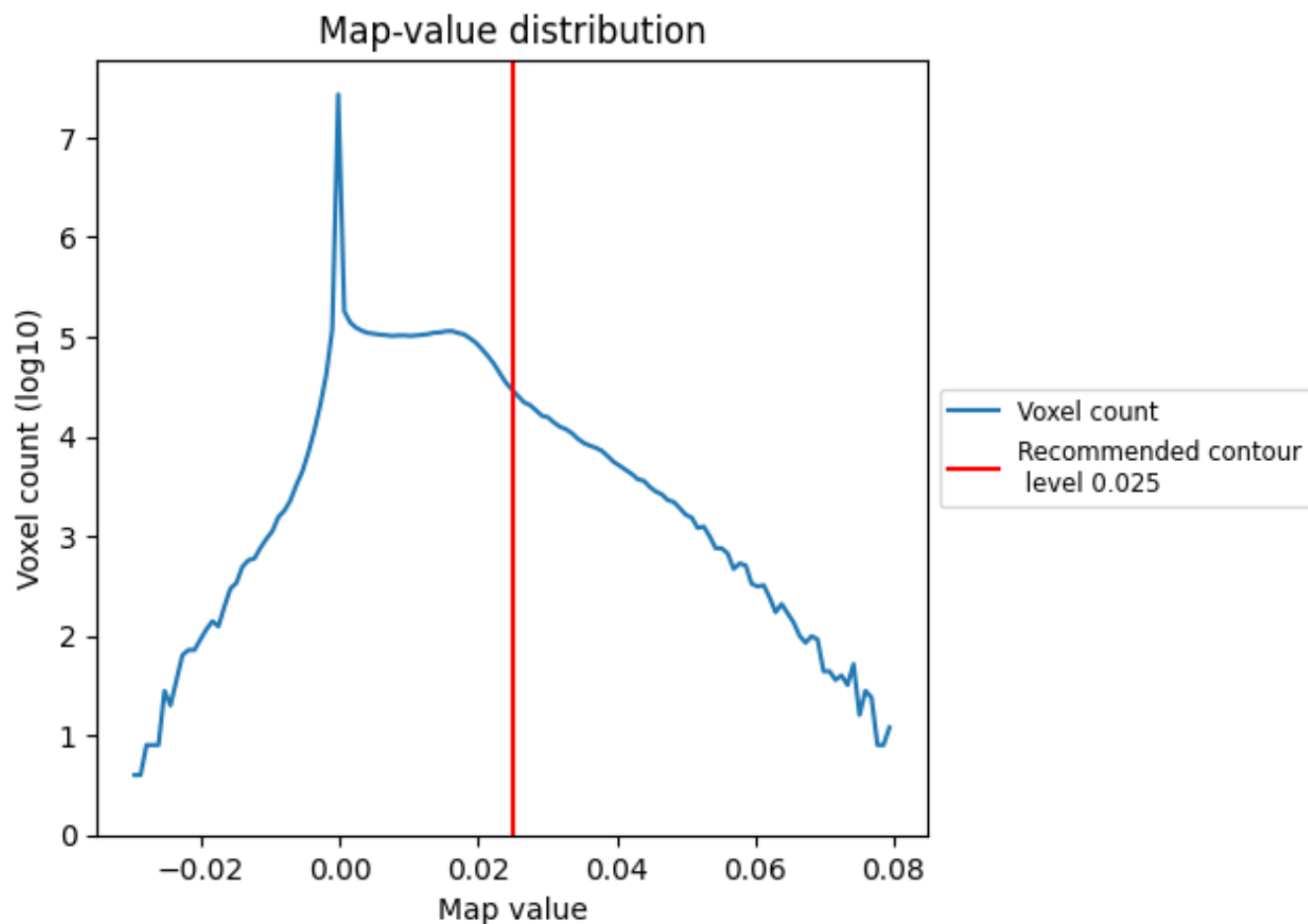
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

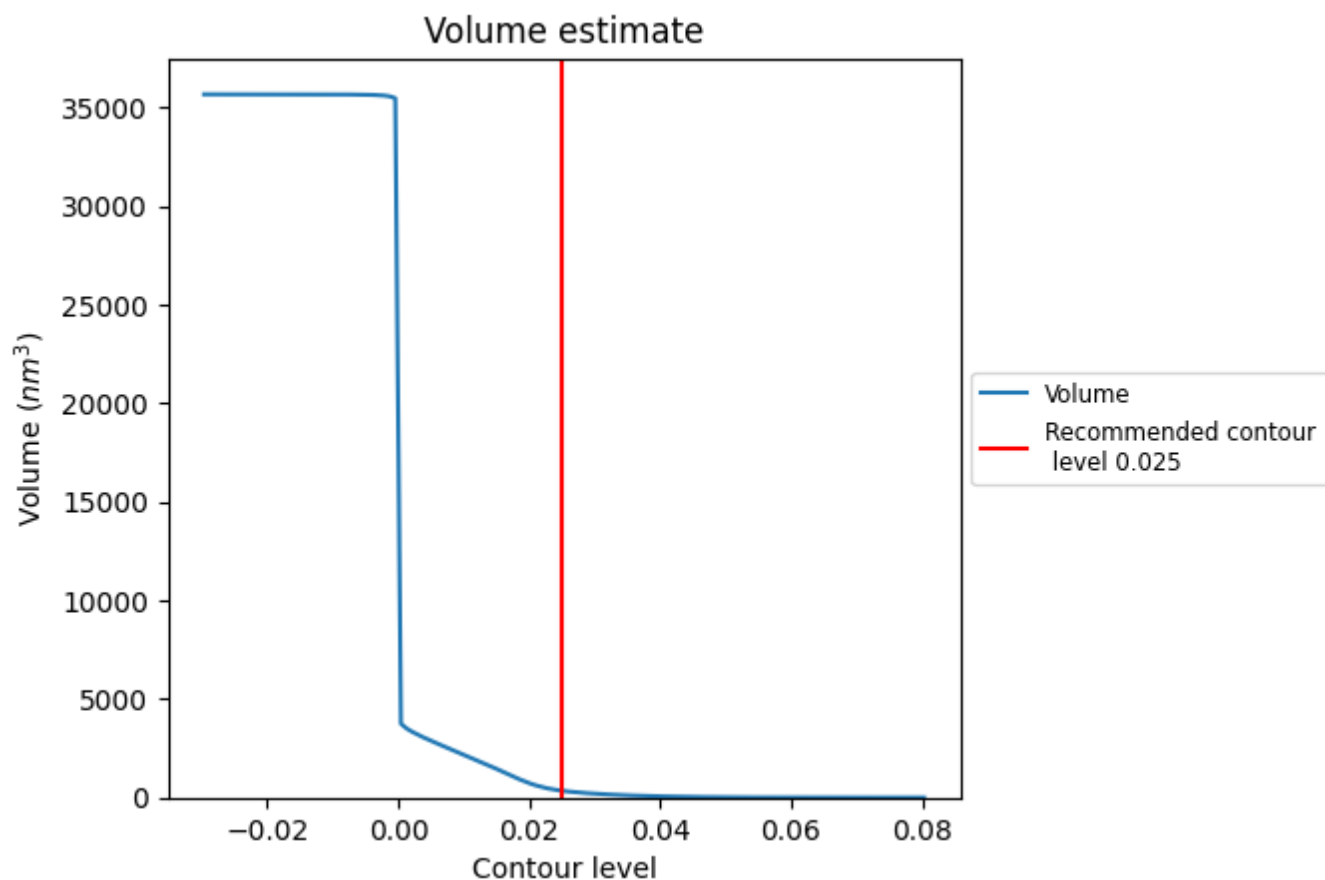
This section contains the results of statistical analysis of the map.

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.

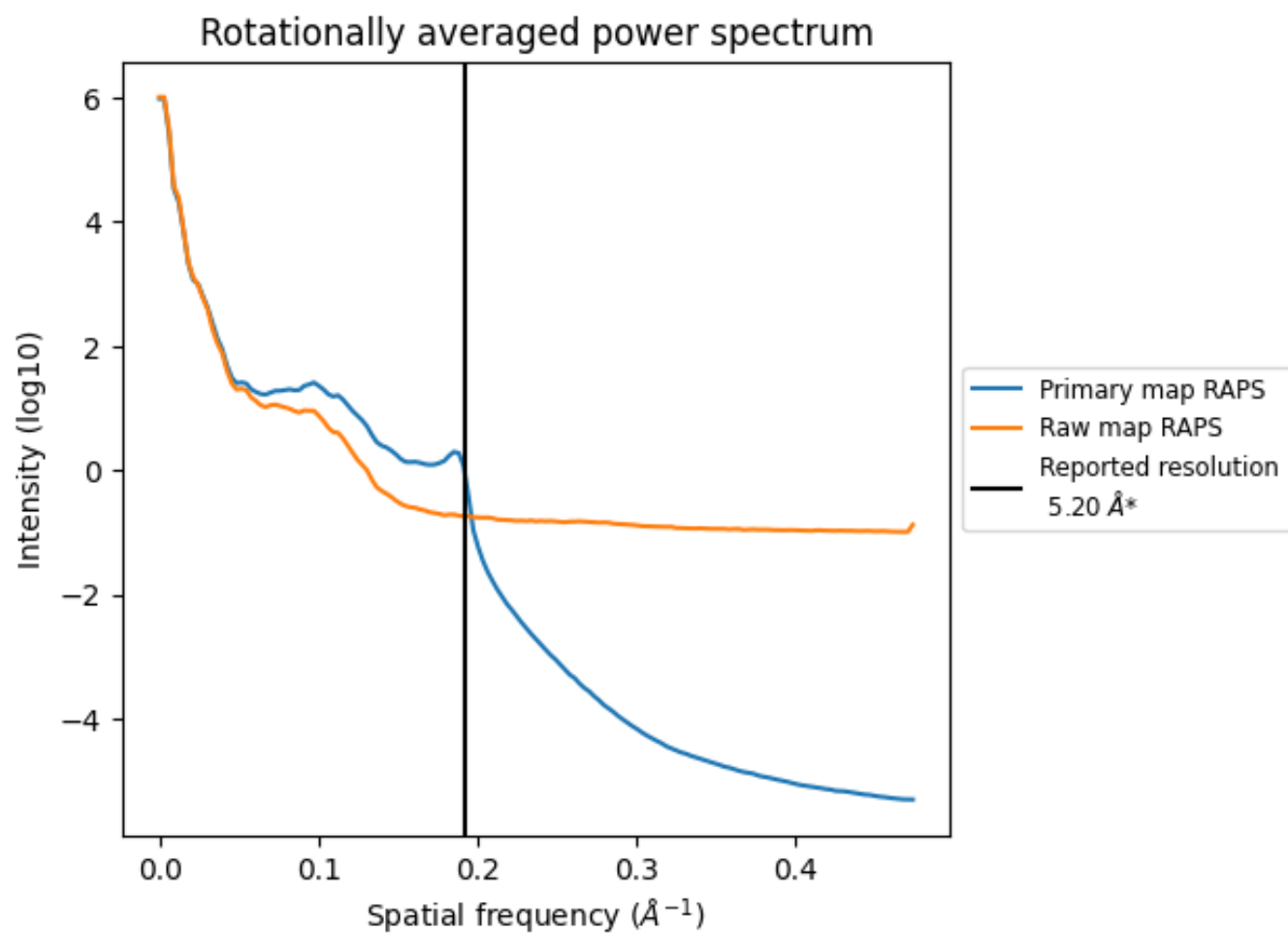
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 347 nm³; this corresponds to an approximate mass of 314 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 ⓘ

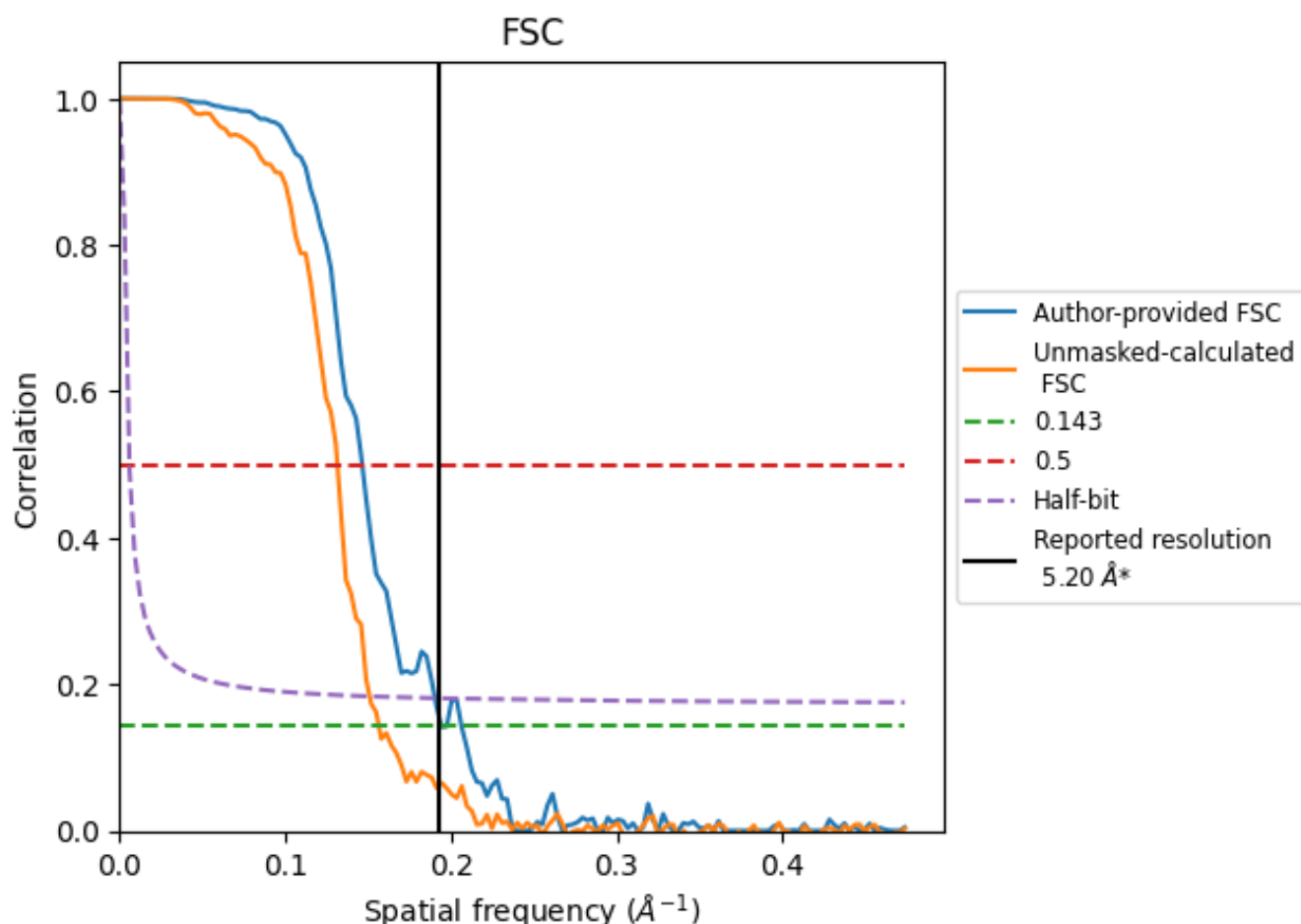


*Reported resolution corresponds to spatial frequency of 0.192 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.192 \AA^{-1}

8.2 Resolution estimates [i](#)

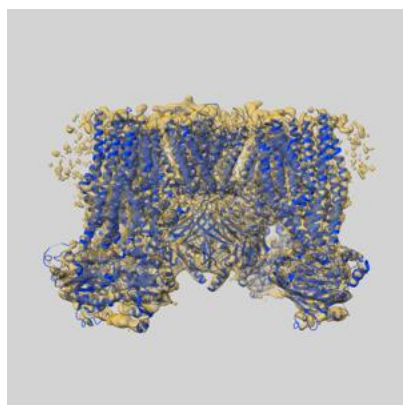
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	5.20	-	-
Author-provided FSC curve	5.15	6.83	5.25
Unmasked-calculated*	6.39	7.60	6.62

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.39 differs from the reported value 5.2 by more than 10 %

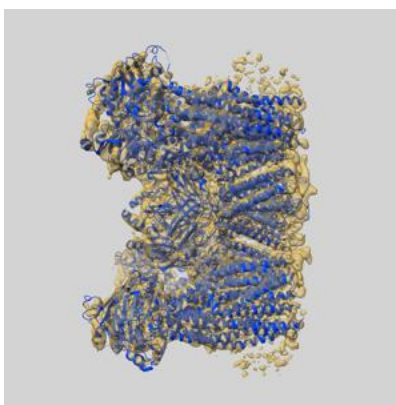
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6851 and PDB model 5YWB. Per-residue inclusion information can be found in section [3](#) on page [6](#).

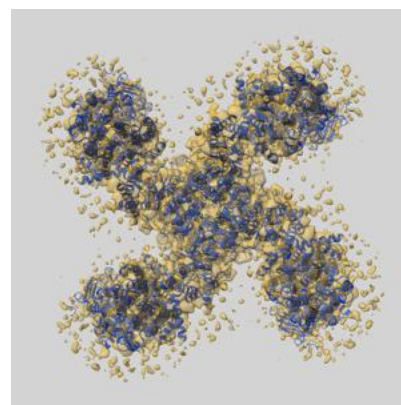
9.1 Map-model overlay [i](#)



X



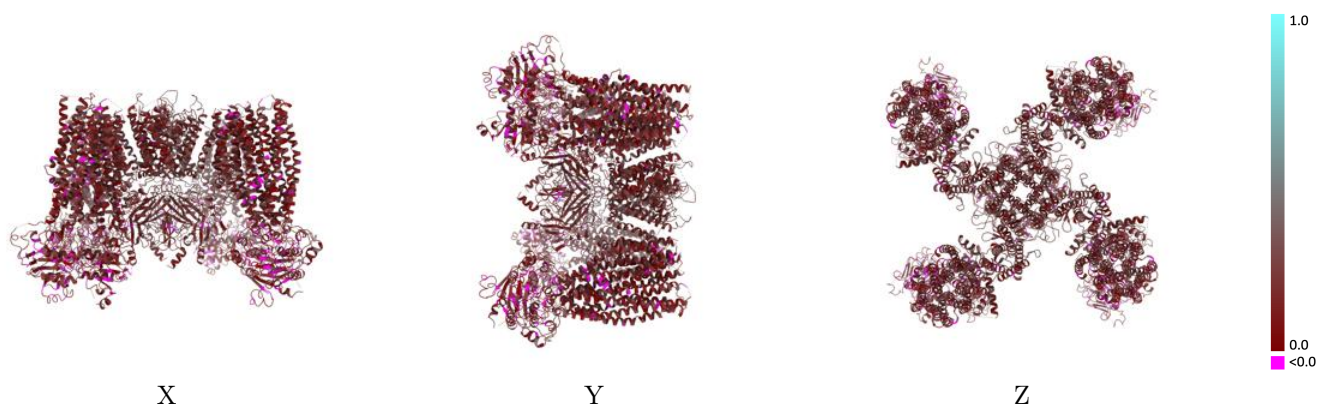
Y



Z

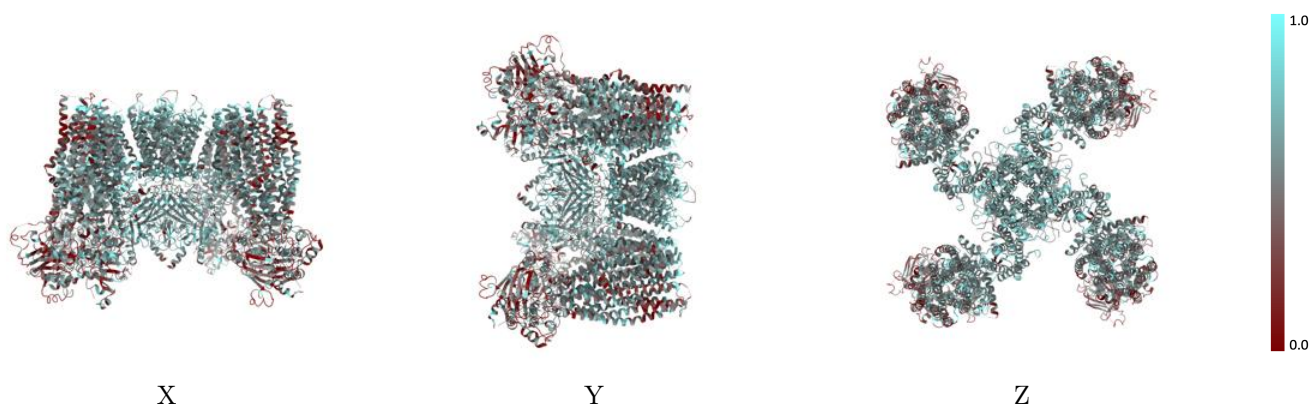
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



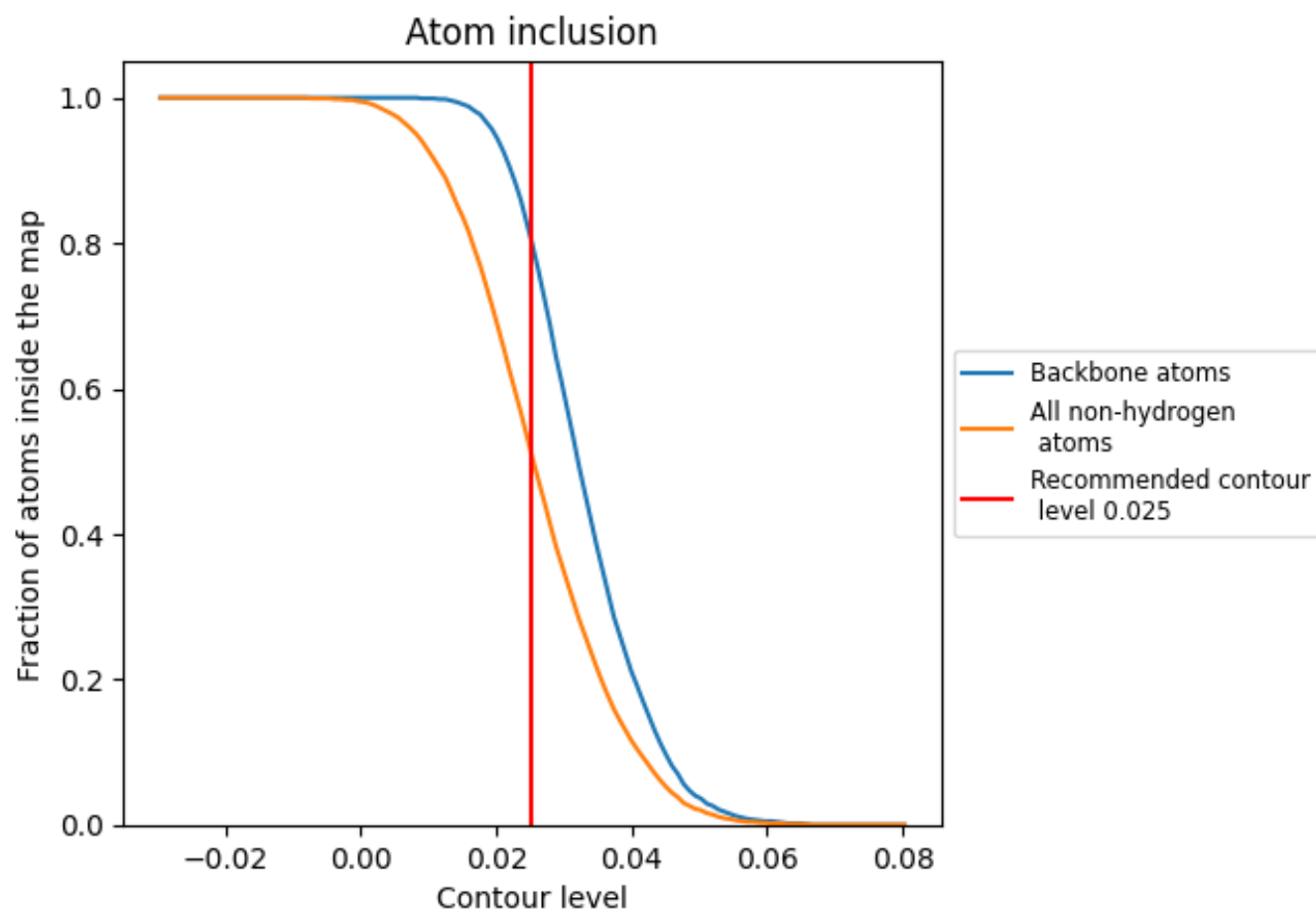
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.025).

9.4 Atom inclusion ⓘ



At the recommended contour level, 81% of all backbone atoms, 52% 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 (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div>0.5160</div>	<div><div></div>0.1930</div>
A	<div><div></div>0.6260</div>	<div><div></div>0.2330</div>
B	<div><div></div>0.4890</div>	<div><div></div>0.1840</div>
C	<div><div></div>0.6260</div>	<div><div></div>0.2350</div>
D	<div><div></div>0.4890</div>	<div><div></div>0.1830</div>
E	<div><div></div>0.6260</div>	<div><div></div>0.2340</div>
F	<div><div></div>0.4890</div>	<div><div></div>0.1830</div>
G	<div><div></div>0.6260</div>	<div><div></div>0.2320</div>
H	<div><div></div>0.4890</div>	<div><div></div>0.1830</div>

1.0

0.0

<0.0