



wwPDB EM Validation Summary Report ⓘ

Nov 11, 2024 – 08:29 AM JST

PDB ID : 5YKF
EMDB ID : EMD-6832
Title : Structure of pancreatic ATP-sensitive potassium channel bound with glibenclamide and ATPgammaS (3D class1 at 4.33Å)
Authors : Chen, L.; Wu, J.X.
Deposited on : 2017-10-14
Resolution : 4.33 Å(reported)

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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

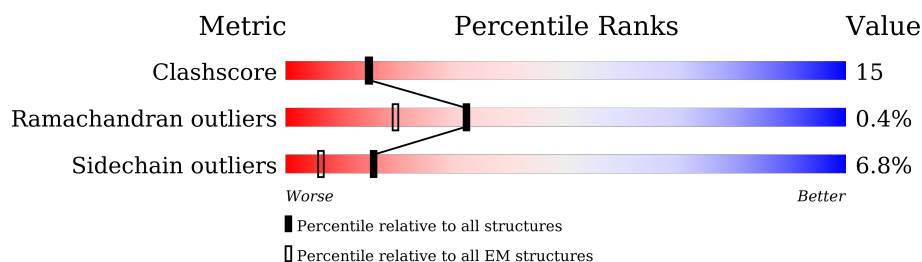
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.33 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	
1	C	390	
1	E	390	
1	G	390	
2	B	1582	
2	D	1582	
2	F	1582	
2	H	1582	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 50988 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.

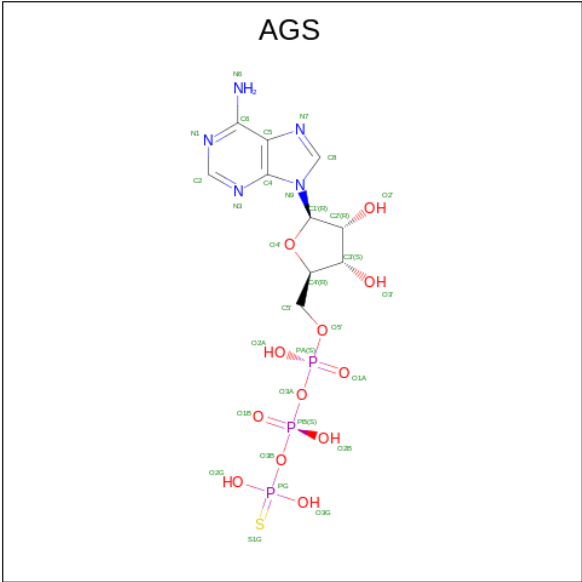
- Molecule 1 is a protein called ATP-sensitive inward rectifier potassium channel 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	325	Total	C	N	O	S	0	0
			2463	1593	426	429	15		
1	C	325	Total	C	N	O	S	0	0
			2463	1593	426	429	15		
1	E	325	Total	C	N	O	S	0	0
			2463	1593	426	429	15		
1	G	325	Total	C	N	O	S	0	0
			2463	1593	426	429	15		

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

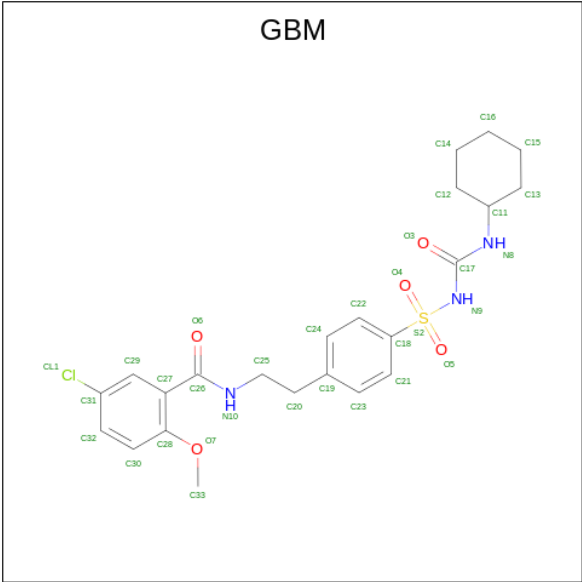
Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1309	Total	C	N	O	S	0	0
			10189	6644	1724	1768	53		
2	D	1309	Total	C	N	O	S	0	0
			10189	6644	1724	1768	53		
2	F	1309	Total	C	N	O	S	0	0
			10189	6644	1724	1768	53		
2	H	1309	Total	C	N	O	S	0	0
			10189	6644	1724	1768	53		

- Molecule 3 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



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

- Molecule 4 is 5-chloro-N-(2-{4-[(cyclohexylcarbamoyl)sulfamoyl]phenyl}ethyl)-2-methoxybenzamide (three-letter code: GBM) (formula: C₂₃H₂₈ClN₃O₅S).

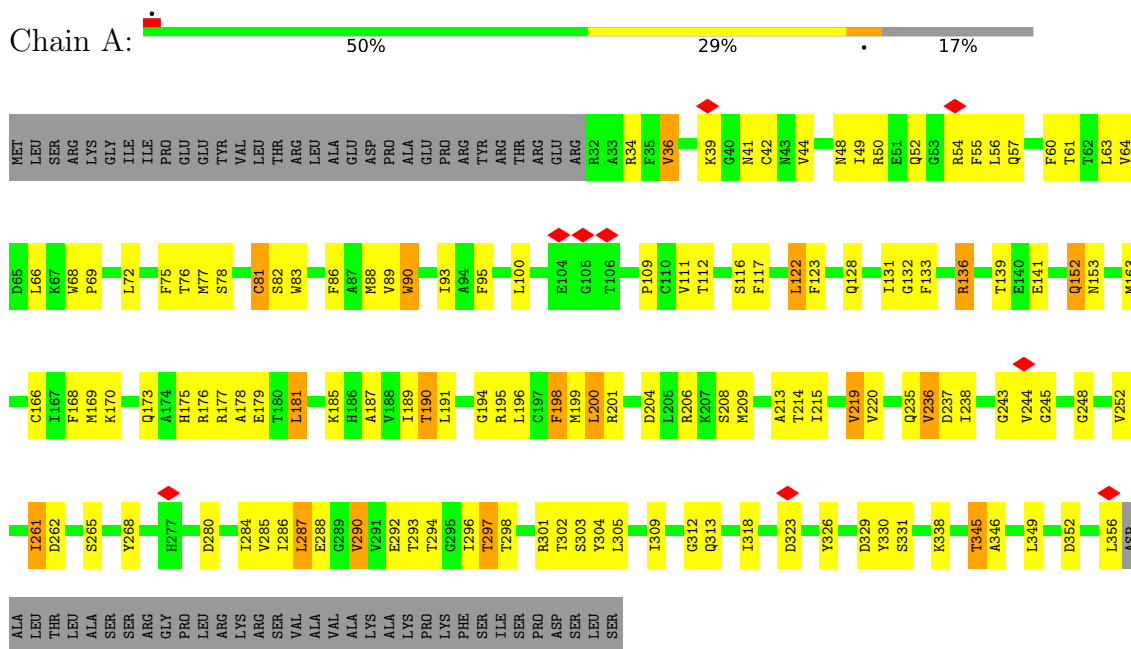


Mol	Chain	Residues	Atoms						AltConf
4	B	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0
4	D	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0
4	F	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0
4	H	1	Total 33	C 23	Cl 1	N 3	O 5	S 1	0

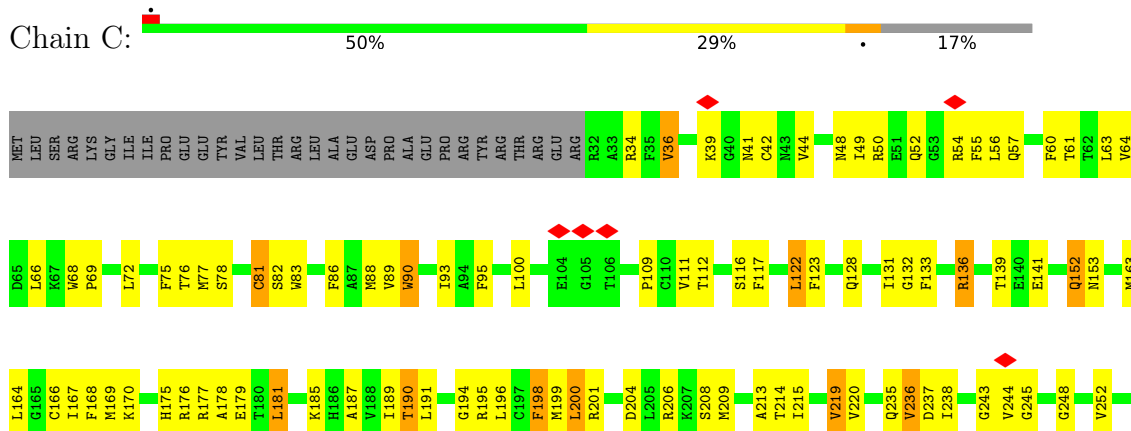
3 Residue-property plots

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.

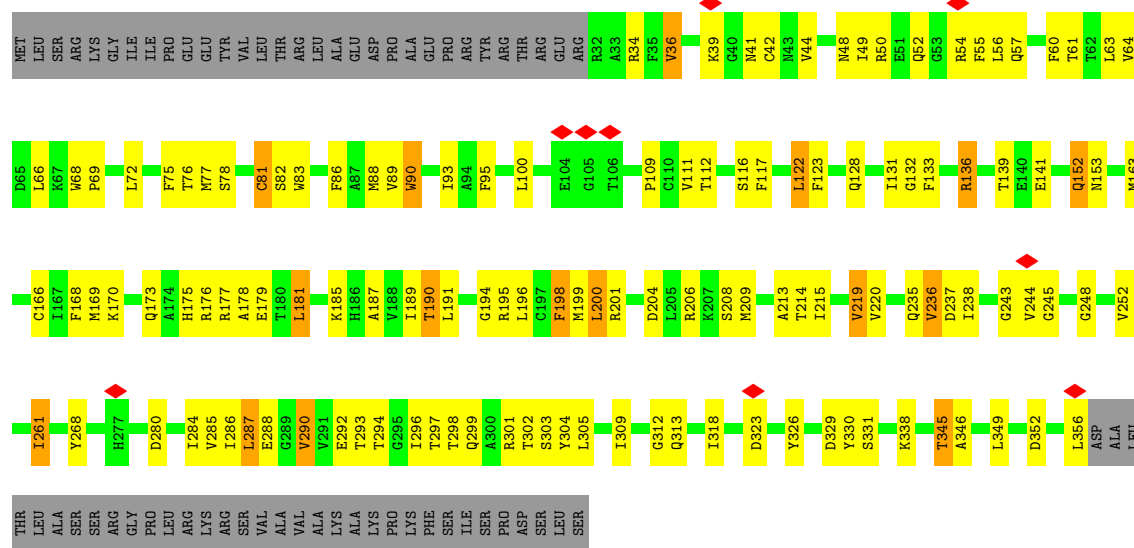
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



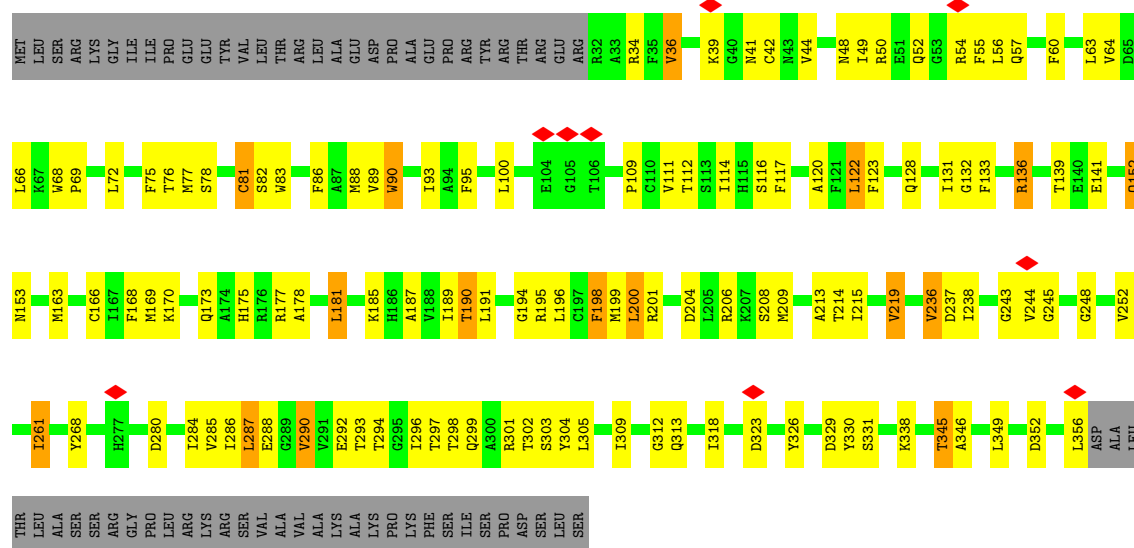
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11



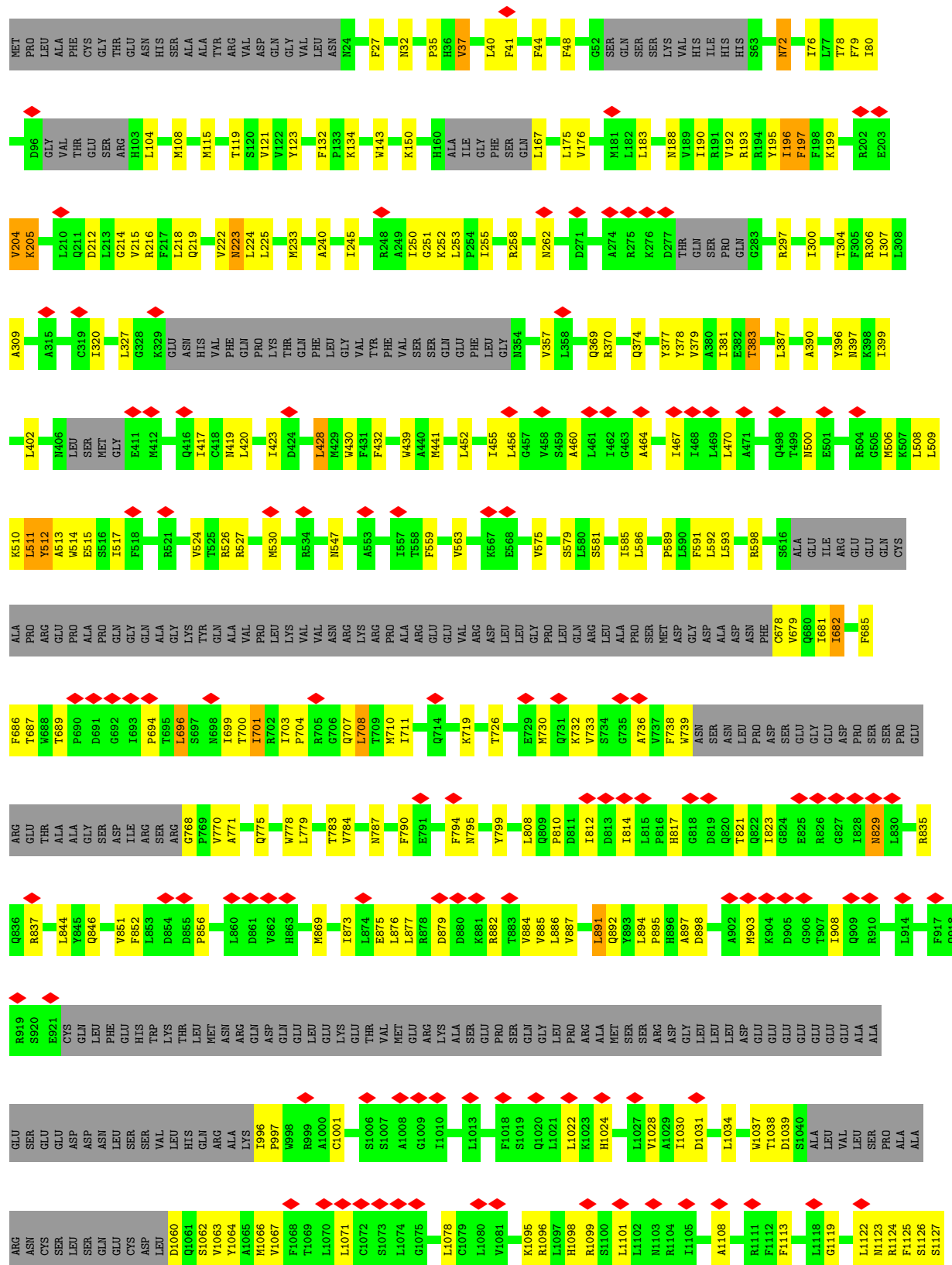
- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

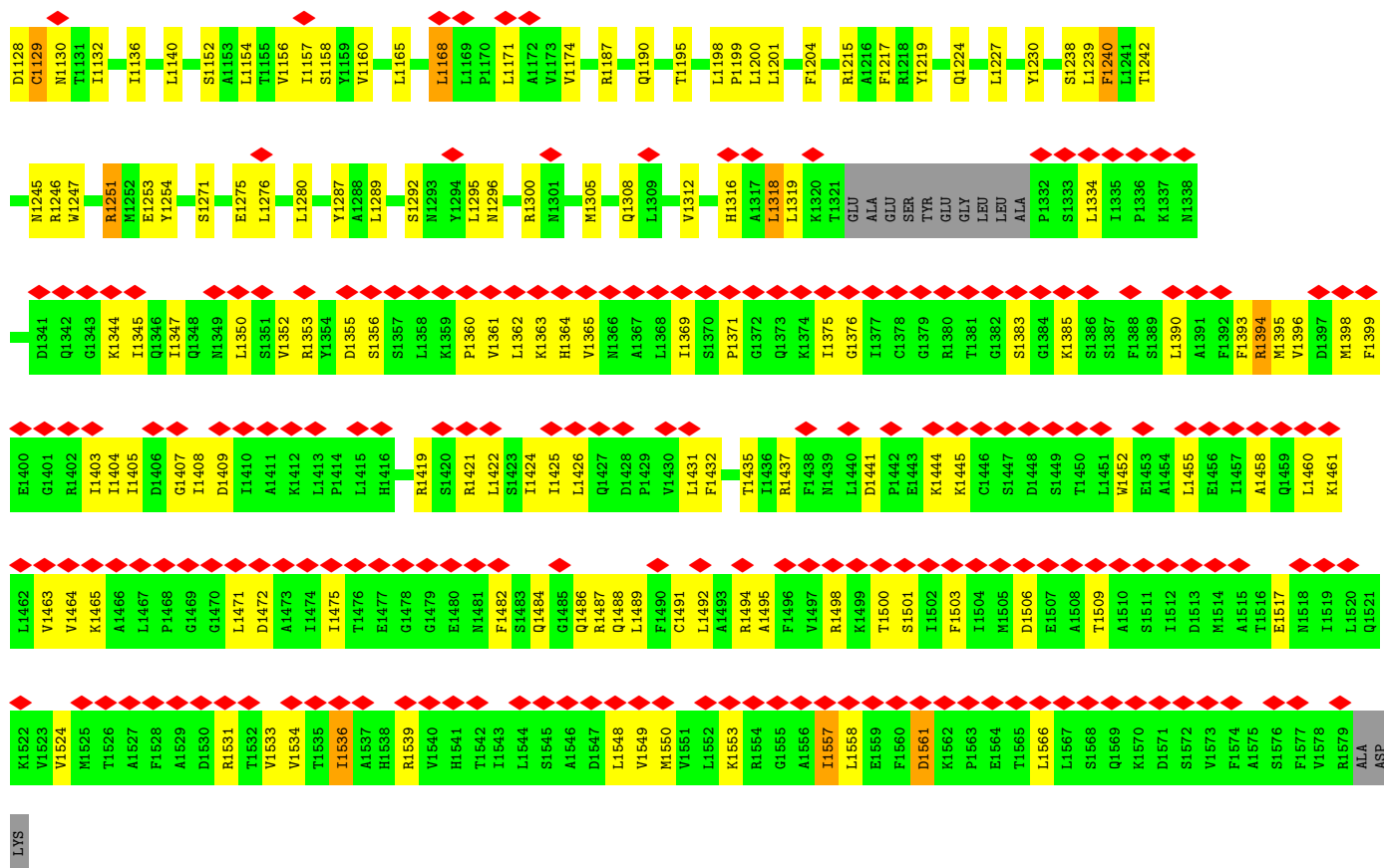


- Molecule 1: ATP-sensitive inward rectifier potassium channel 11

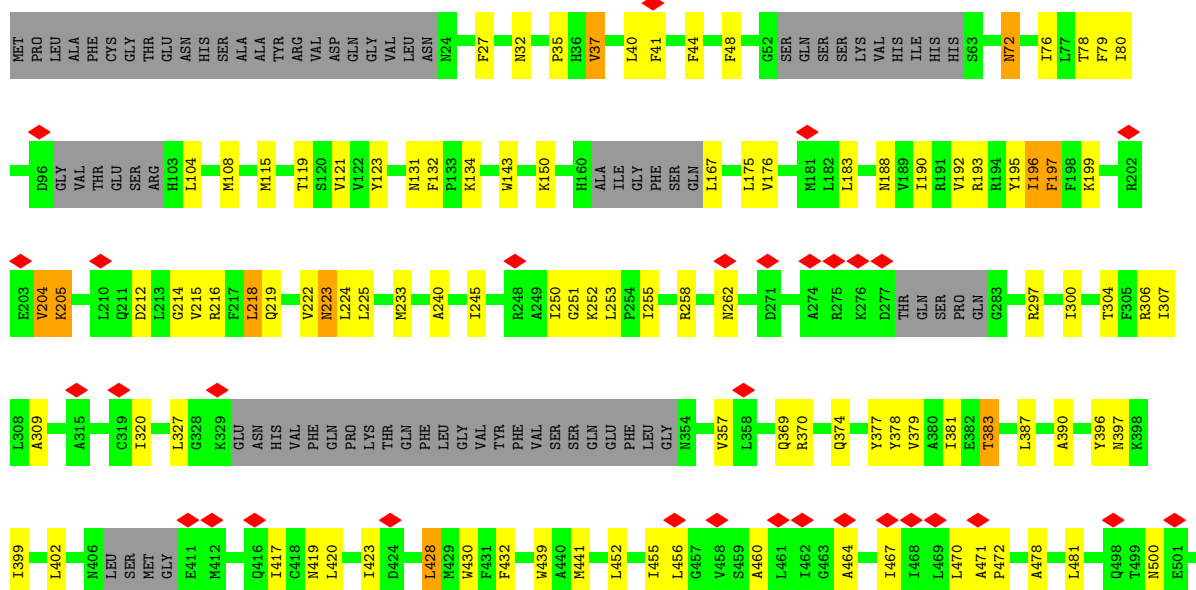


- Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2



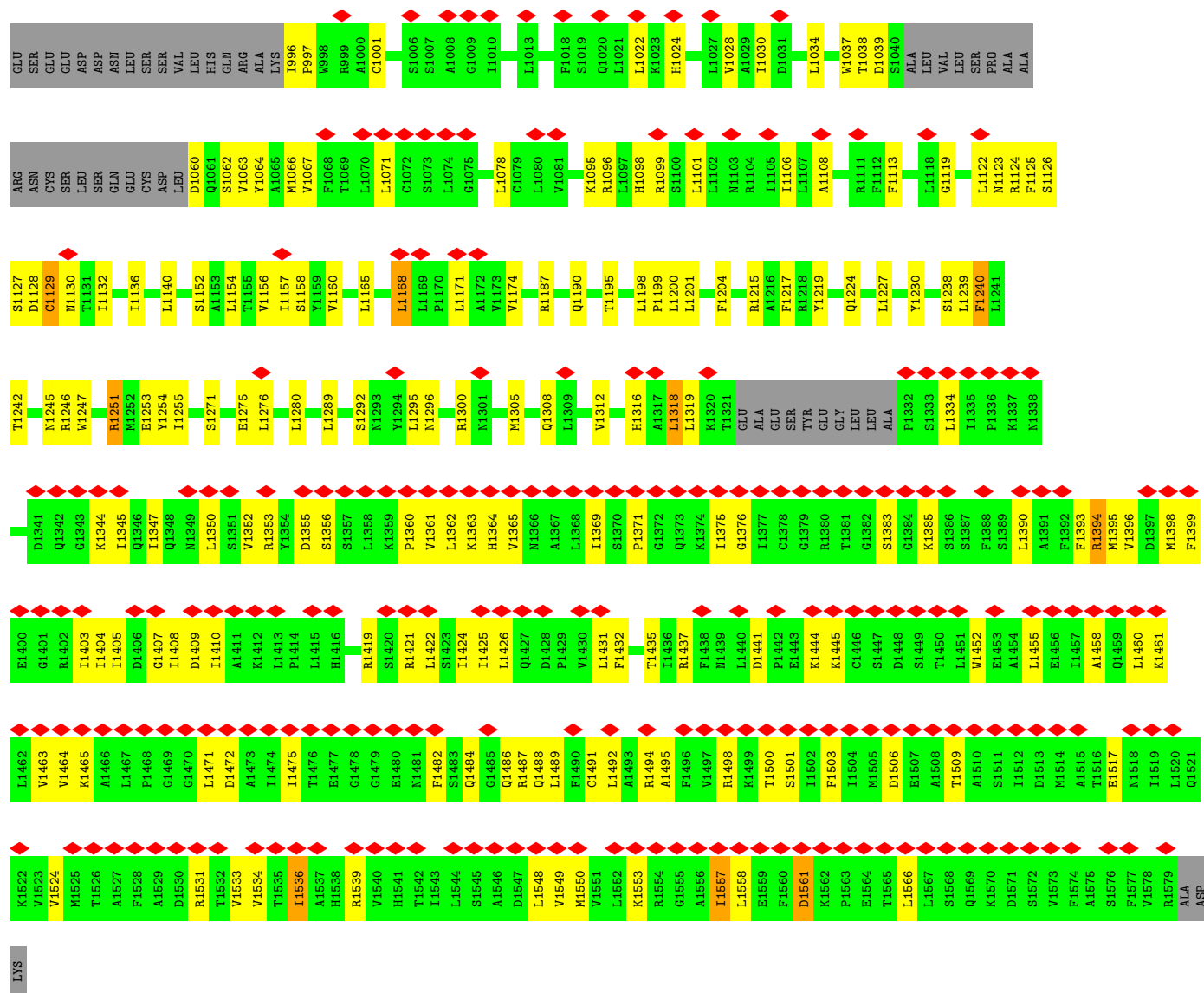


• Molecule 2: ATP-binding cassette sub-family C member 8 isoform X2

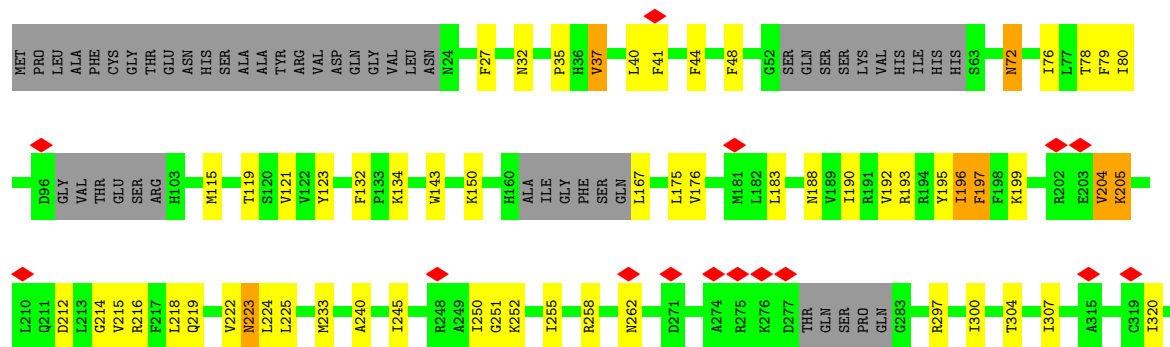


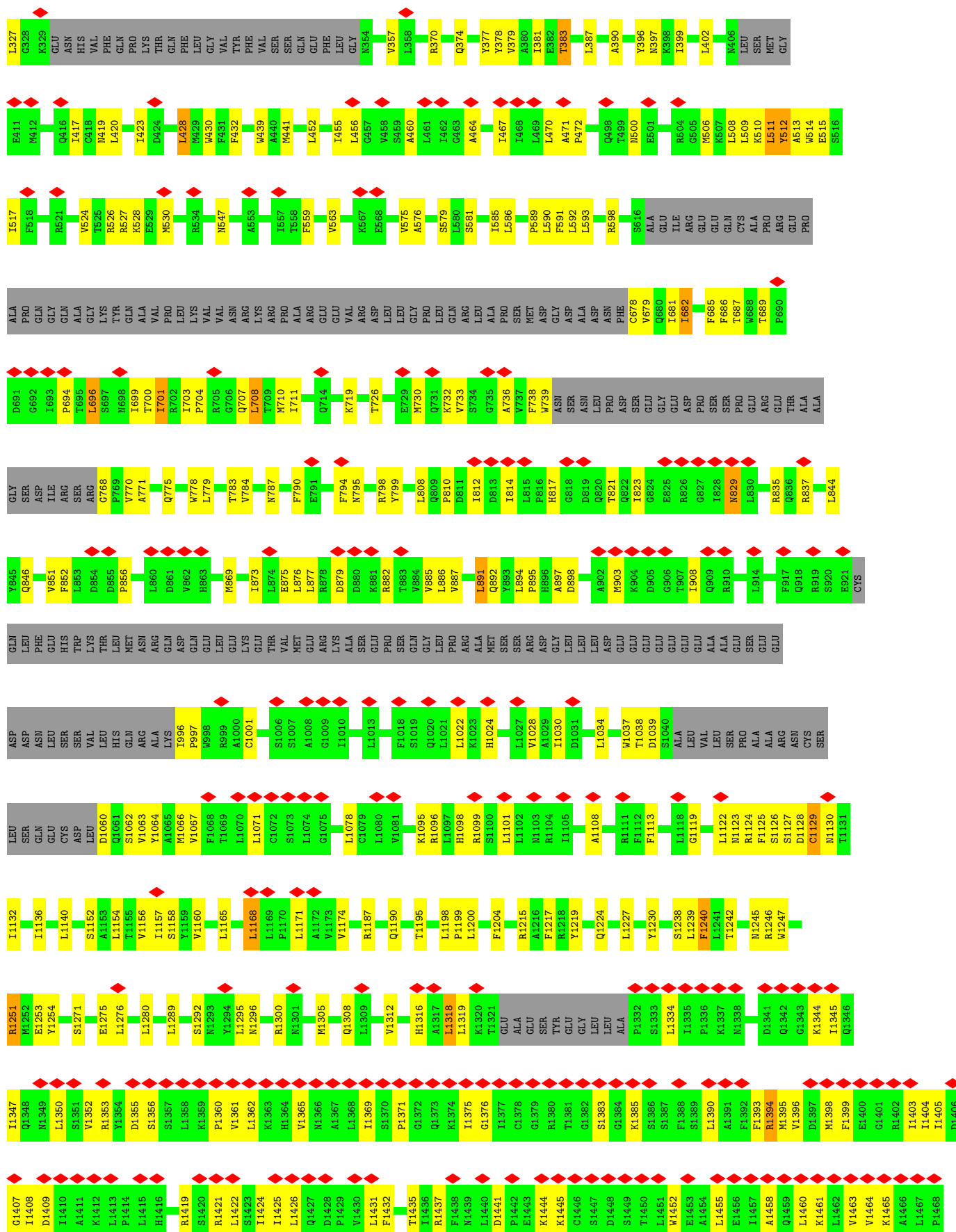
Q1459	D1397	F1240	R1124	Q909	R826	C678	R504
L1460	M1398	L1241	F1125	R910	Q827	V679	G505
K1461	F1399	T1242	GLU	L914	T828	Q680	M506
L1462	E1400	N1245	GLU	F917	N829	I682	K507
V1463	G1401	R1246	ALA	Q918	L830	F685	L508
V1464	R1402	W1247	ALA	R919	R835	F686	L509
K1465	I1403	R1251	GLU	Q918	R836	T687	K510
A1466	I1404	M1252	GLU	R919	R836	W688	L511
A1466	I1405	E1253	CYS	S920	R837	T689	A513
L1467	D1406	Y1254	GLU	E921	L844	F690	W514
P1468	G1407	S1271	ASP	CYS	Y845	D691	E515
G1469	I1408	E1275	ASN	GLN	Q846	G692	S516
G1470	D1409	L1276	LEU	PHE	W851	G692	I517
D1471	I1410	L1276	GLU	GLU	F852	I693	F518
D1472	A1411	L1280	TRP	HIS	L853	P694	R521
A1473	K1412	V1156	LYS	TRP	D854	T695	V524
I1474	L1413	Y1287	LYS	THR	D855	S697	T525
I1475	P1414	S1158	LEU	THR	P856	N698	R526
T1476	L1415	V1159	LEU	LEU	W770	T700	R527
E1477	H1416	L1289	ARG	MET	L860	I701	M530
G1478	R1419	S1292	ASN	ASN	D861	R702	R534
G1479	S1420	N1293	GLN	ASP	W778	I703	R534
E1480	R1421	Y1294	ASP	GLN	L779	P704	N647
N1481	L1422	L1295	GLU	GLU	T783	R705	A553
F1482	L1423	N1296	LEU	LEU	V784	G706	I557
S1483	S1424	R1300	GLY	LYS	N869	L708	F559
Q1484	I1424	N1301	GLU	THR	I873	T709	V663
G1485	I1425	V1172	THR	VAL	L874	I711	K567
R1487	L1426	V1174	VAL	GLU	E875	W710	E568
Q1487	Q1427	V1174	MET	GLU	L876	F790	V575
Q1488	D1428	L1080	GLU	GLU	L877	E791	A576
L1489	L1429	V1081	ARG	LYS	R878	F794	S579
F1490	V1430	K1095	LYS	LYS	D879	N795	L580
C1491	L1431	R1096	ALA	ALA	D880	Y799	S581
L1492	F1432	L1097	GLU	SER	K881	T726	I585
A1493	H1316	H1098	PRO	GLU	R882	E729	L586
A1494	A1317	R1099	SER	SER	T883	W730	P589
A1495	L1318	R1099	SER	GLN	V884	Q731	L590
F1496	L1319	S1100	GLY	GLY	V885	K732	F591
V1497	K1320	L1101	LEU	LEU	L886	W733	L593
F1497	T1321	L1102	PRO	PRO	V887	S734	R598
R1498	GLU	M1103	ARG	ALA	L891	G735	S616
R1499	ALA	R1104	ALA	MET	Q892	A736	ALA
R1500	GLU	I1105	MET	SER	T893	V737	
S1501	TYR	L1106	SER	SER	L894	F738	
I1502	GLY	A1108	ARG	ARG	P895	W739	
F1503	GLY	Q1224	ASP	ASP	H896	Q818	
C1446	LEU	L1227	GLY	GLY	A897	D819	
S1447	LEU	L1227	LEU	LEU	D898	Q820	
D1448	ALA	Y1230	LEU	LEU	A902	T821	
D1449	P1332	S1238	ASP	ASP	M903	L823	
T1450	S1333	L1334	GLU	GLU	R904	G824	
L1451	L1334	I1336	GLU	GLU	D905	E825	
A1510	I1336				T907		
E1453					I908		
A1511							
I1512							
D1513							
M1514							
A1515							
T1516							
E1517							
N1518							





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







4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	27322	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	0.088	Depositor
Minimum map value	-0.047	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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.38	0/2518	0.55	0/3430
1	C	0.38	0/2518	0.55	0/3430
1	E	0.38	0/2518	0.55	0/3430
1	G	0.38	0/2518	0.55	0/3430
2	B	0.28	0/10394	0.45	0/14113
2	D	0.28	0/10394	0.45	0/14113
2	F	0.28	0/10394	0.45	0/14113
2	H	0.28	0/10394	0.45	0/14113
All	All	0.30	0/51648	0.47	0/70172

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 [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	2463	0	2451	106	0
1	C	2463	0	2451	104	0
1	E	2463	0	2451	105	0
1	G	2463	0	2451	104	0
2	B	10189	0	10510	294	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	10189	0	10510	290	0
2	F	10189	0	10510	291	0
2	H	10189	0	10510	288	0
3	A	62	0	24	10	0
3	B	31	0	12	2	0
3	C	31	0	12	5	0
3	D	31	0	12	2	0
3	E	31	0	12	5	0
3	F	31	0	12	2	0
3	H	31	0	12	2	0
4	B	33	0	28	4	0
4	D	33	0	28	4	0
4	F	33	0	28	3	0
4	H	33	0	28	3	0
All	All	50988	0	52052	1537	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 15.

The worst 5 of 1537 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:200:LEU:HD12	1:G:201:ARG:N	1.51	1.25
1:A:200:LEU:HD12	1:A:201:ARG:N	1.51	1.25
1:C:200:LEU:HD12	1:C:201:ARG:N	1.51	1.22
1:E:200:LEU:HD12	1:E:201:ARG:N	1.51	1.22
1:A:200:LEU:CD1	1:A:201:ARG:N	2.05	1.20

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%)	304 (94%)	18 (6%)	1 (0%)	37	72
1	C	323/390 (83%)	304 (94%)	18 (6%)	1 (0%)	37	72
1	E	323/390 (83%)	304 (94%)	18 (6%)	1 (0%)	37	72
1	G	323/390 (83%)	304 (94%)	18 (6%)	1 (0%)	37	72
2	B	1285/1582 (81%)	1226 (95%)	53 (4%)	6 (0%)	25	63
2	D	1285/1582 (81%)	1226 (95%)	53 (4%)	6 (0%)	25	63
2	F	1285/1582 (81%)	1226 (95%)	53 (4%)	6 (0%)	25	63
2	H	1285/1582 (81%)	1226 (95%)	53 (4%)	6 (0%)	25	63
All	All	6432/7888 (82%)	6120 (95%)	284 (4%)	28 (0%)	32	67

5 of 28 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	197	PHE
2	B	199	LYS
2	D	197	PHE
2	D	199	LYS
2	F	197	PHE

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	258/339 (76%)	226 (88%)	32 (12%)	4	17
1	C	258/339 (76%)	226 (88%)	32 (12%)	4	17
1	E	258/339 (76%)	226 (88%)	32 (12%)	4	17
1	G	258/339 (76%)	226 (88%)	32 (12%)	4	17
2	B	1102/1371 (80%)	1041 (94%)	61 (6%)	18	41
2	D	1102/1371 (80%)	1041 (94%)	61 (6%)	18	41
2	F	1102/1371 (80%)	1041 (94%)	61 (6%)	18	41
2	H	1102/1371 (80%)	1041 (94%)	61 (6%)	18	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	5440/6840 (80%)	5068 (93%)	372 (7%)	16	34

5 of 372 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	374	GLN
1	G	111	VAL
2	F	470	LEU
2	F	1238	SER
1	G	238	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 33 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	152	GLN
1	G	173	GLN
2	H	485	GLN
1	C	152	GLN
1	C	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](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AGS	H	2002	-	26,33,33	1.89	4 (15%)	26,52,52	1.47	4 (15%)
4	GBM	H	2001	-	35,35,35	2.02	4 (11%)	48,48,48	1.87	7 (14%)
4	GBM	F	2001	-	35,35,35	2.02	4 (11%)	48,48,48	1.87	7 (14%)
3	AGS	B	2002	-	26,33,33	1.89	4 (15%)	26,52,52	1.47	4 (15%)
3	AGS	A	401	-	26,33,33	2.30	3 (11%)	26,52,52	1.60	7 (26%)
4	GBM	D	2001	-	35,35,35	2.02	4 (11%)	48,48,48	1.87	7 (14%)
3	AGS	A	402	-	26,33,33	2.30	3 (11%)	26,52,52	1.60	7 (26%)
3	AGS	D	2002	-	26,33,33	1.89	4 (15%)	26,52,52	1.47	4 (15%)
3	AGS	C	401	-	26,33,33	2.30	3 (11%)	26,52,52	1.60	7 (26%)
3	AGS	E	401	-	26,33,33	2.30	3 (11%)	26,52,52	1.60	7 (26%)
3	AGS	F	2002	-	26,33,33	1.89	4 (15%)	26,52,52	1.47	4 (15%)
4	GBM	B	2001	-	35,35,35	2.02	4 (11%)	48,48,48	1.87	7 (14%)

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	AGS	H	2002	-	-	2/17/38/38	0/3/3/3
4	GBM	H	2001	-	-	8/27/35/35	0/3/3/3
4	GBM	F	2001	-	-	8/27/35/35	0/3/3/3
3	AGS	B	2002	-	-	2/17/38/38	0/3/3/3
3	AGS	A	401	-	-	5/17/38/38	0/3/3/3
4	GBM	D	2001	-	-	8/27/35/35	0/3/3/3
3	AGS	A	402	-	-	5/17/38/38	0/3/3/3
3	AGS	D	2002	-	-	2/17/38/38	0/3/3/3
3	AGS	C	401	-	-	5/17/38/38	0/3/3/3
3	AGS	E	401	-	-	5/17/38/38	0/3/3/3
3	AGS	F	2002	-	-	2/17/38/38	0/3/3/3
4	GBM	B	2001	-	-	8/27/35/35	0/3/3/3

The worst 5 of 44 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	401	AGS	PG-S1G	10.12	2.12	1.90
3	A	402	AGS	PG-S1G	10.12	2.12	1.90
3	C	401	AGS	PG-S1G	10.12	2.12	1.90
3	E	401	AGS	PG-S1G	10.12	2.12	1.90
4	B	2001	GBM	C18-S2	-10.08	1.60	1.76

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2001	GBM	O5-S2-O4	-9.71	107.62	119.55
4	D	2001	GBM	O5-S2-O4	-9.71	107.62	119.55
4	F	2001	GBM	O5-S2-O4	-9.71	107.62	119.55
4	H	2001	GBM	O5-S2-O4	-9.71	107.62	119.55
4	B	2001	GBM	O7-C28-C27	3.75	122.01	116.55

There are no chirality outliers.

5 of 60 torsion outliers are listed below:

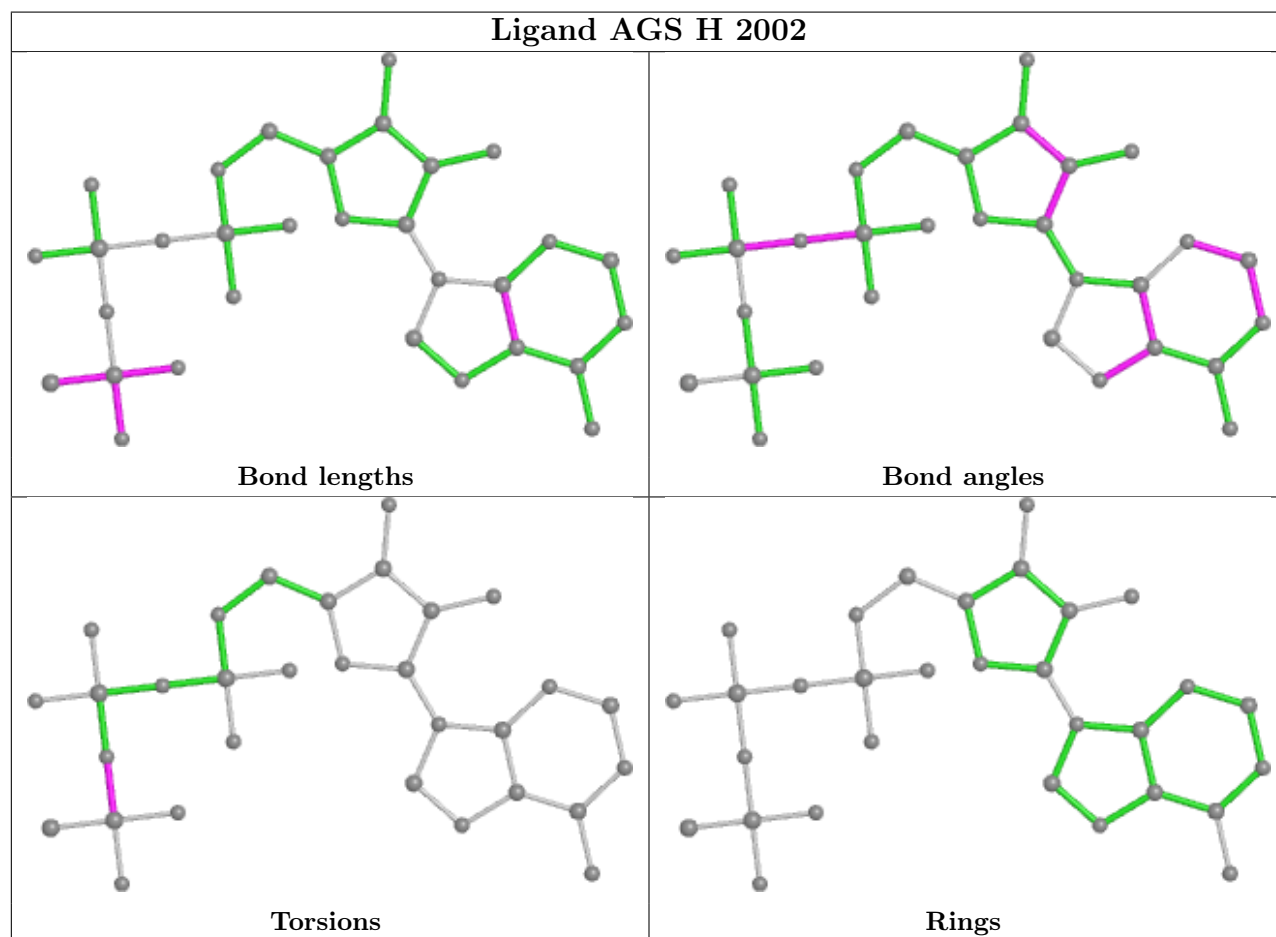
Mol	Chain	Res	Type	Atoms
3	B	2002	AGS	PB-O3B-PG-O2G
3	B	2002	AGS	PB-O3B-PG-O3G
3	D	2002	AGS	PB-O3B-PG-O2G
3	D	2002	AGS	PB-O3B-PG-O3G
3	F	2002	AGS	PB-O3B-PG-O2G

There are no ring outliers.

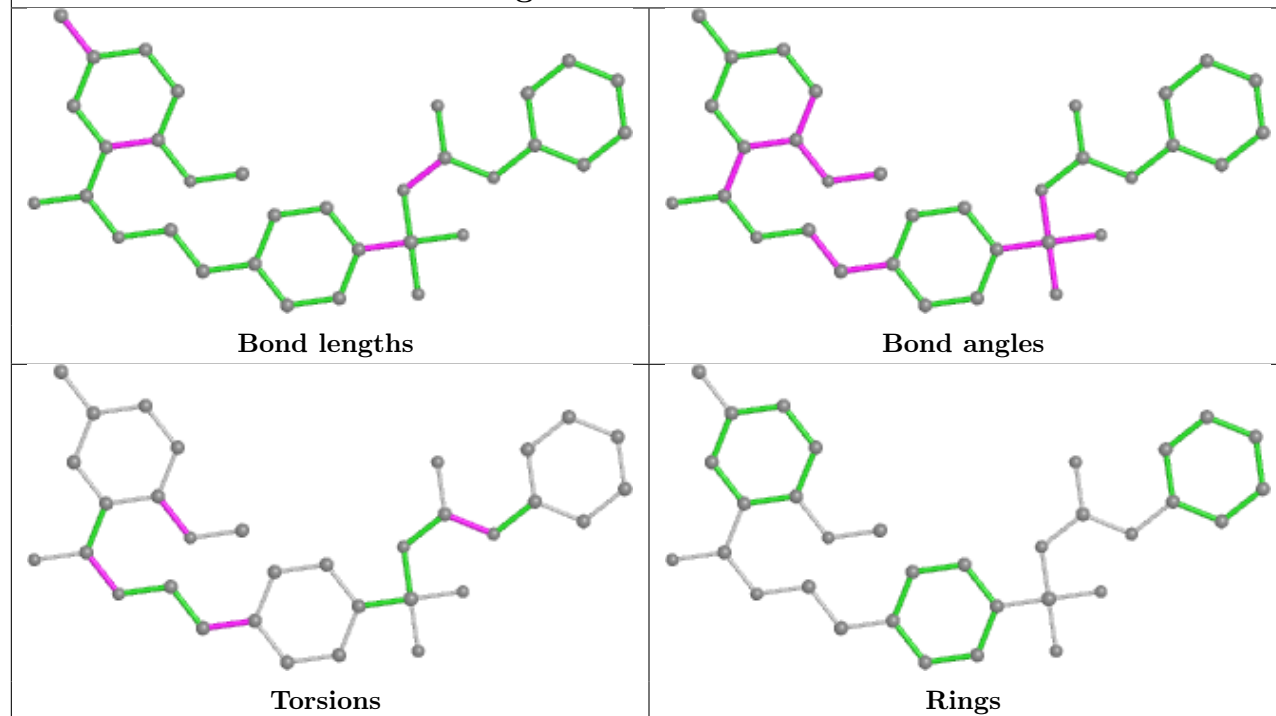
12 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	H	2002	AGS	2	0
4	H	2001	GBM	3	0
4	F	2001	GBM	3	0
3	B	2002	AGS	2	0
3	A	401	AGS	5	0
4	D	2001	GBM	4	0
3	A	402	AGS	5	0
3	D	2002	AGS	2	0
3	C	401	AGS	5	0
3	E	401	AGS	5	0
3	F	2002	AGS	2	0
4	B	2001	GBM	4	0

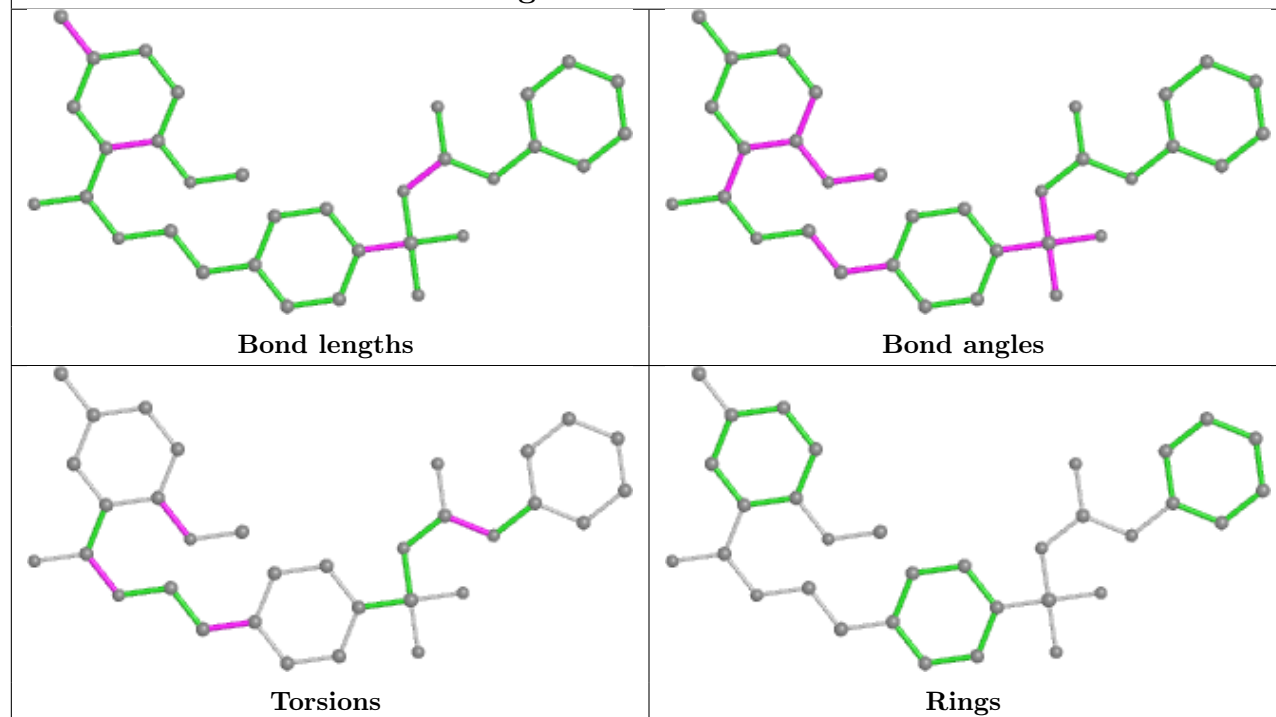
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

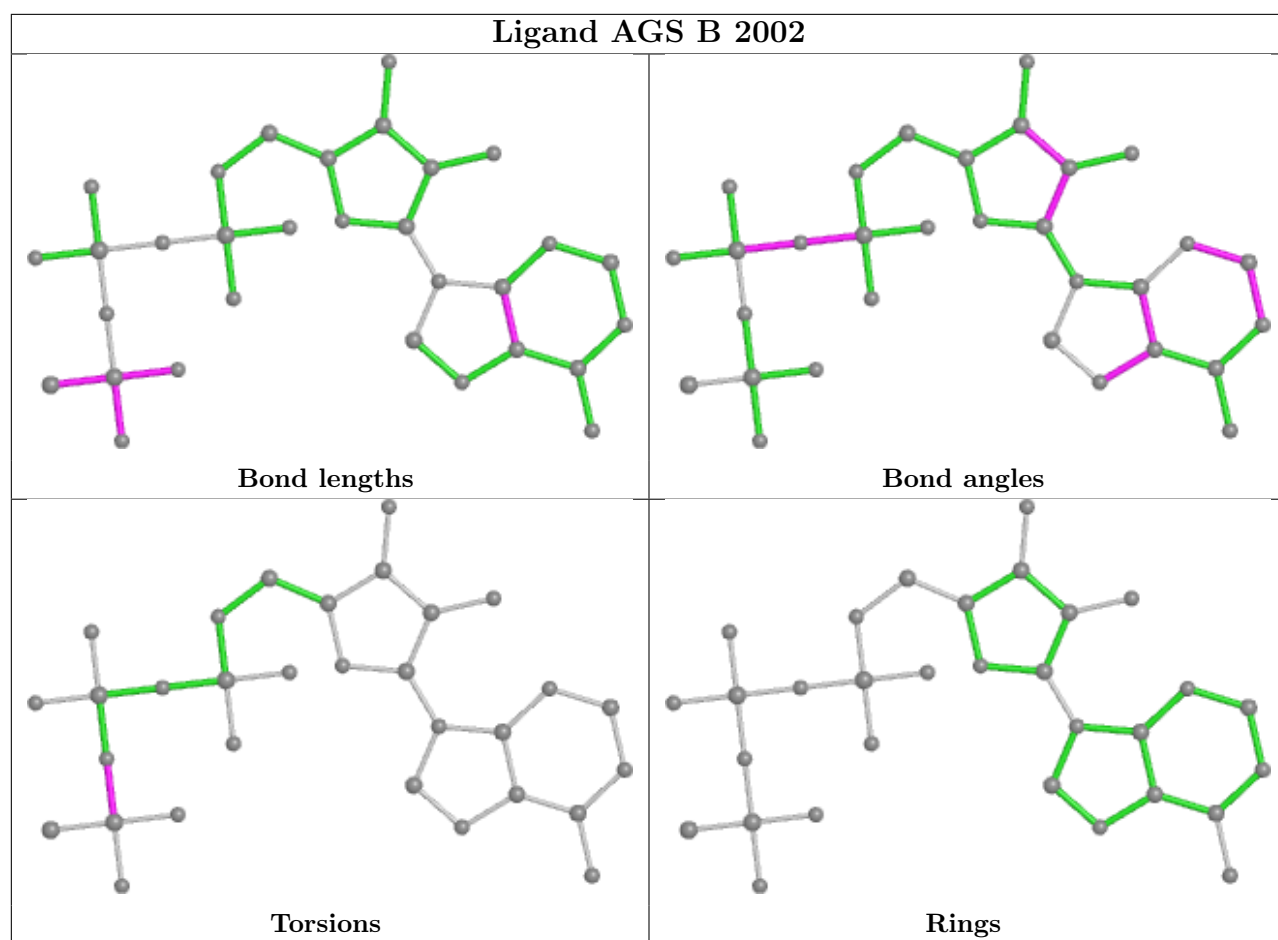


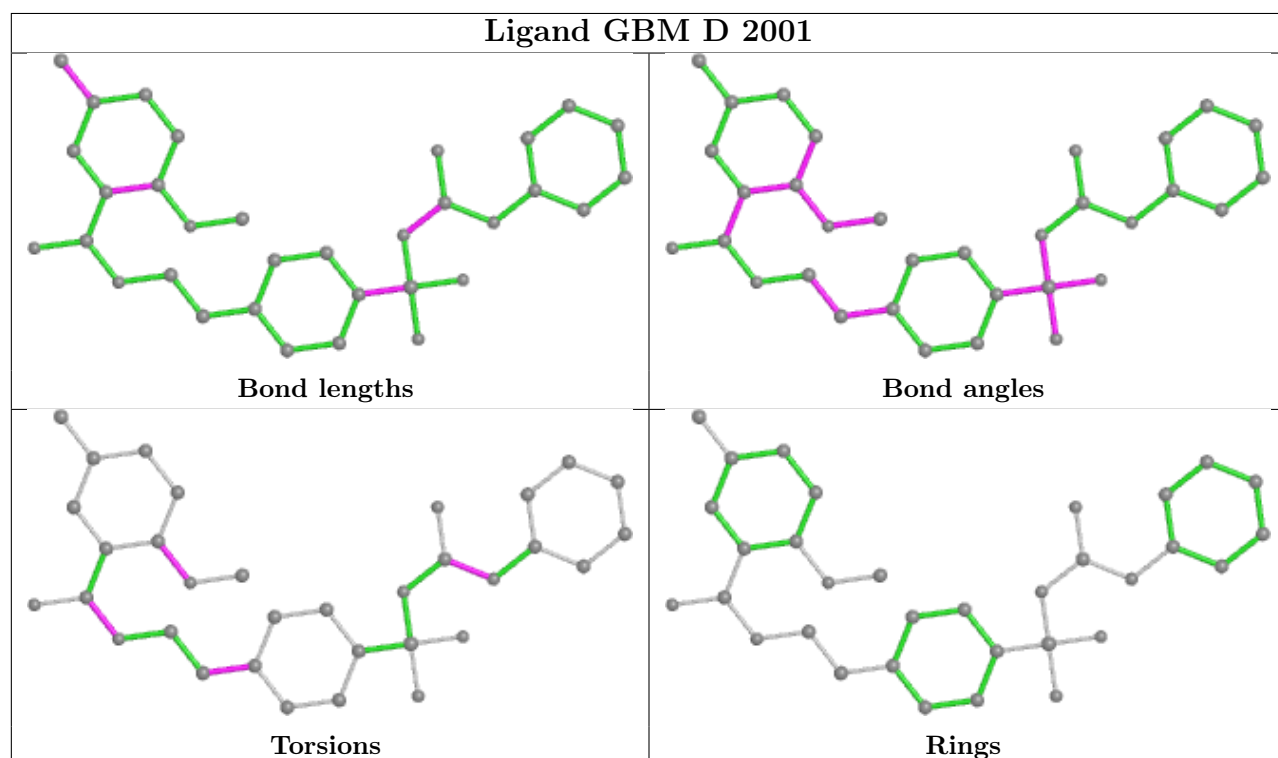
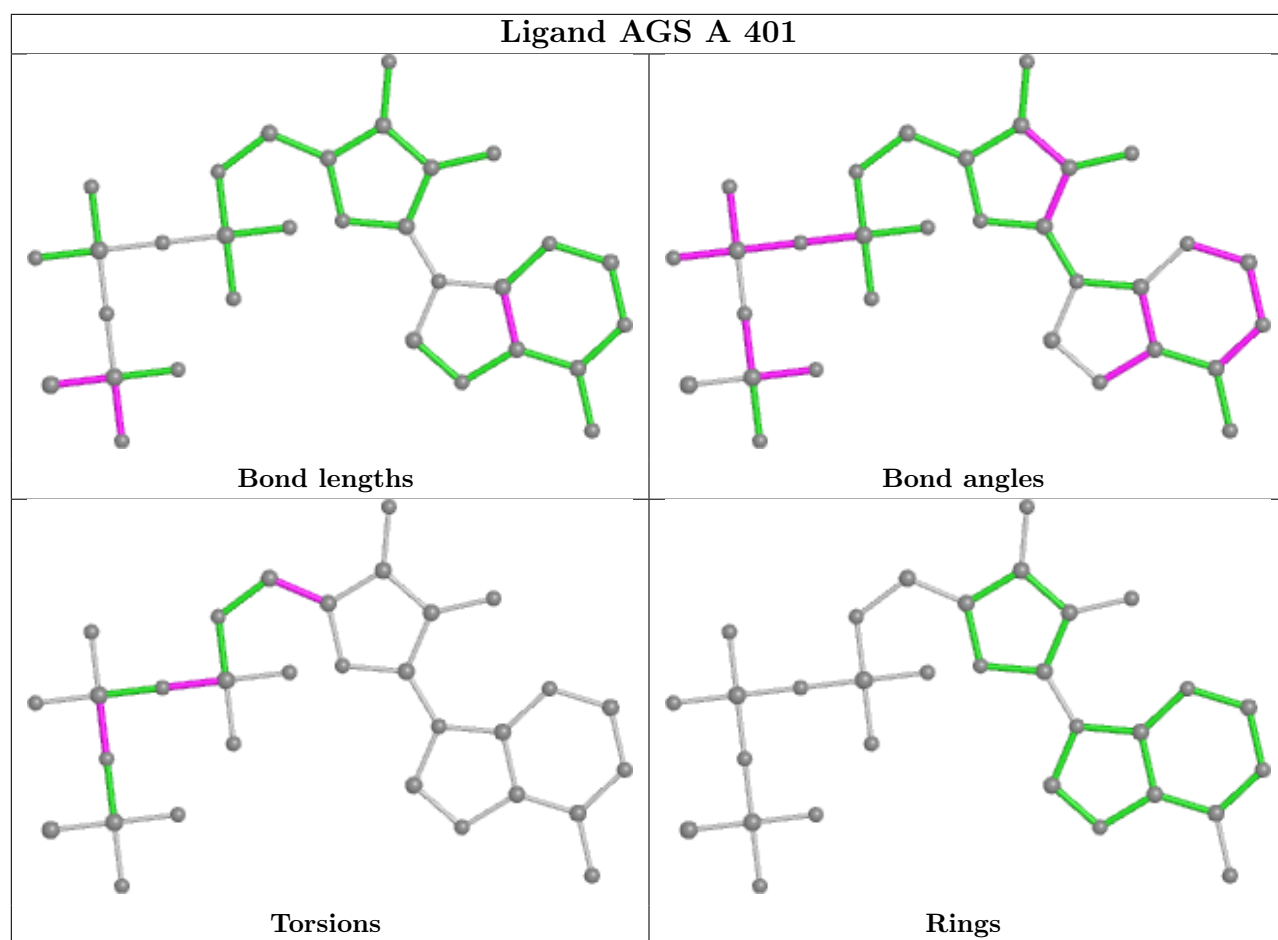
Ligand GBM H 2001

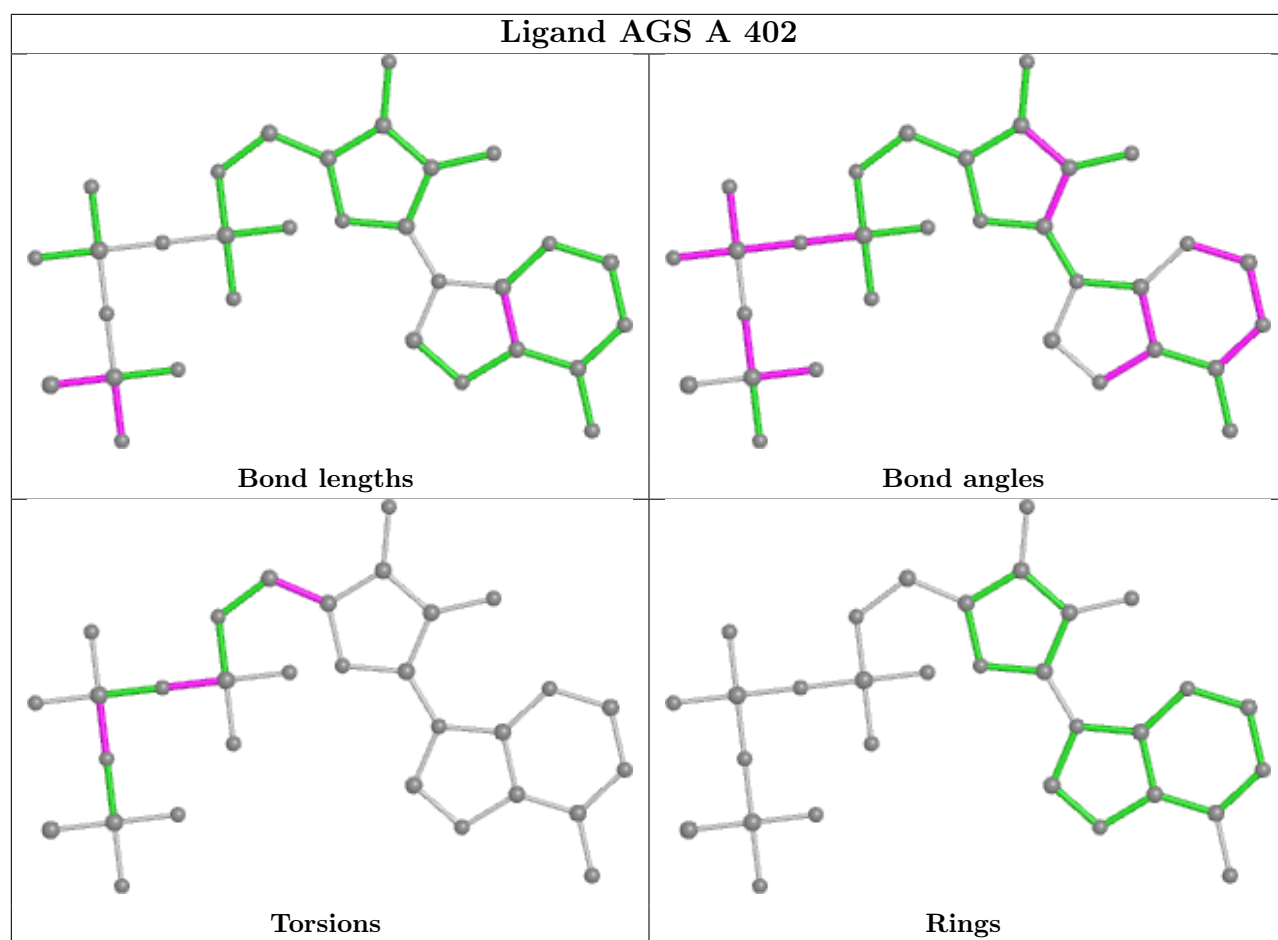


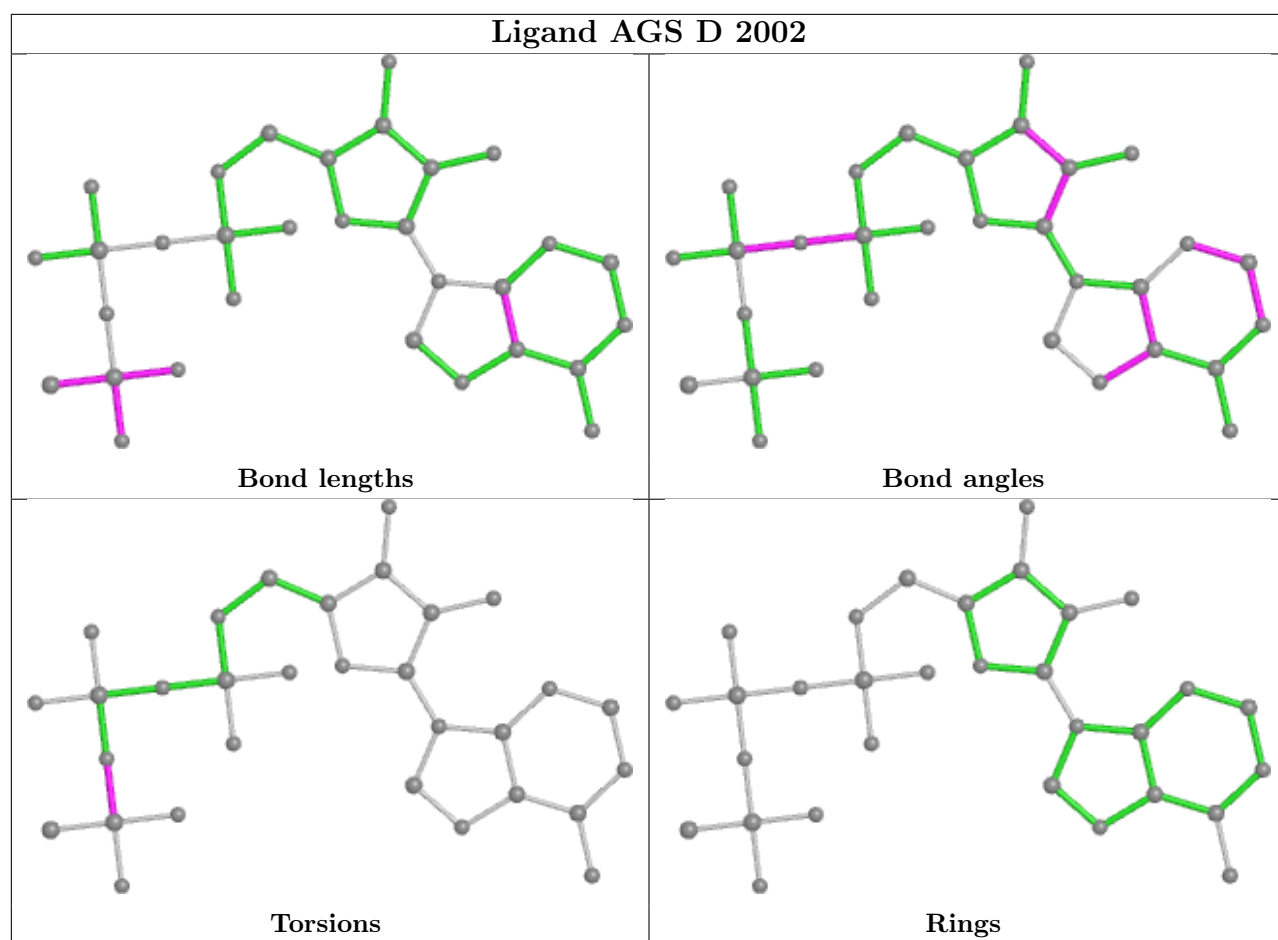
Ligand GBM F 2001

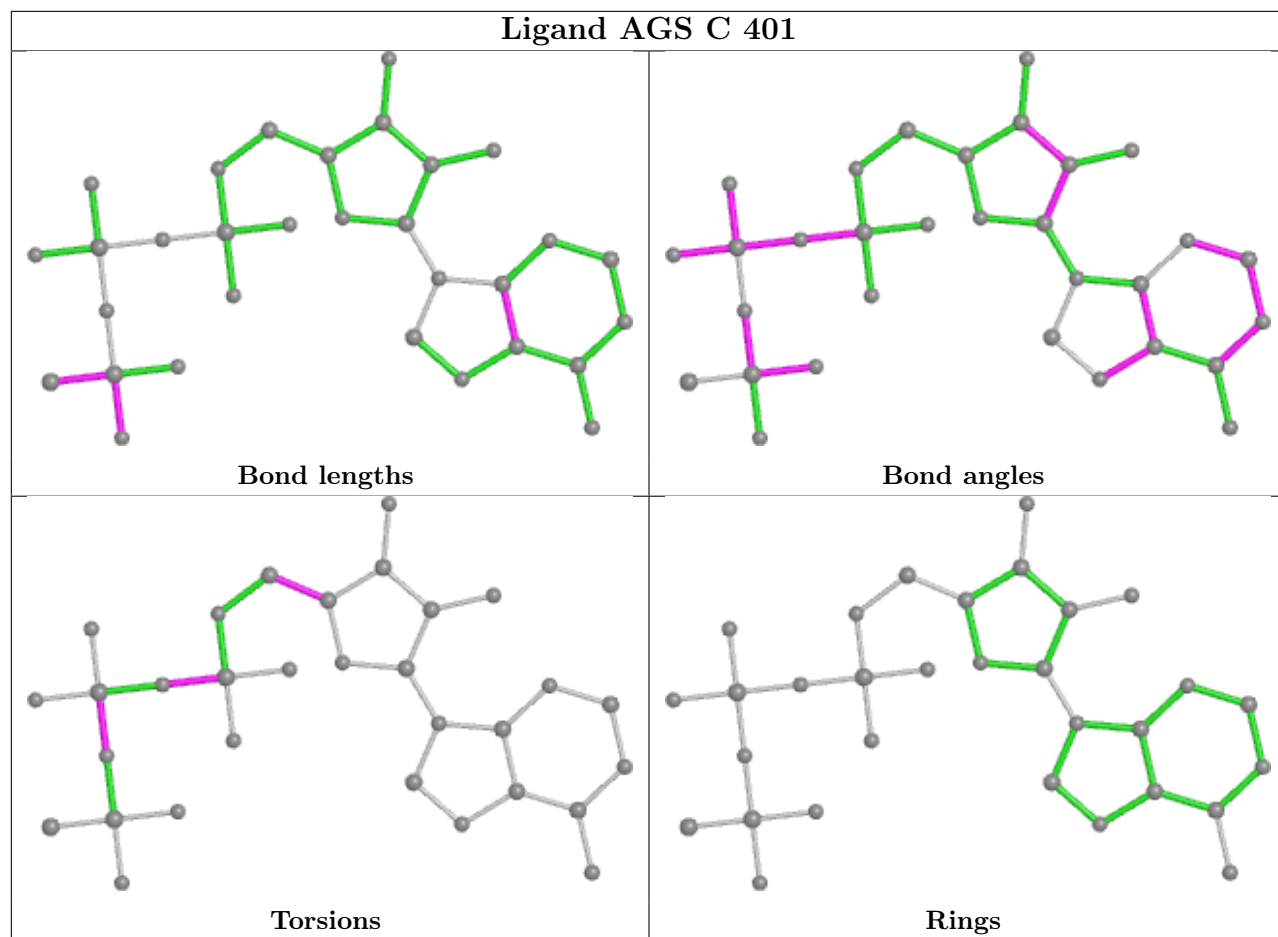




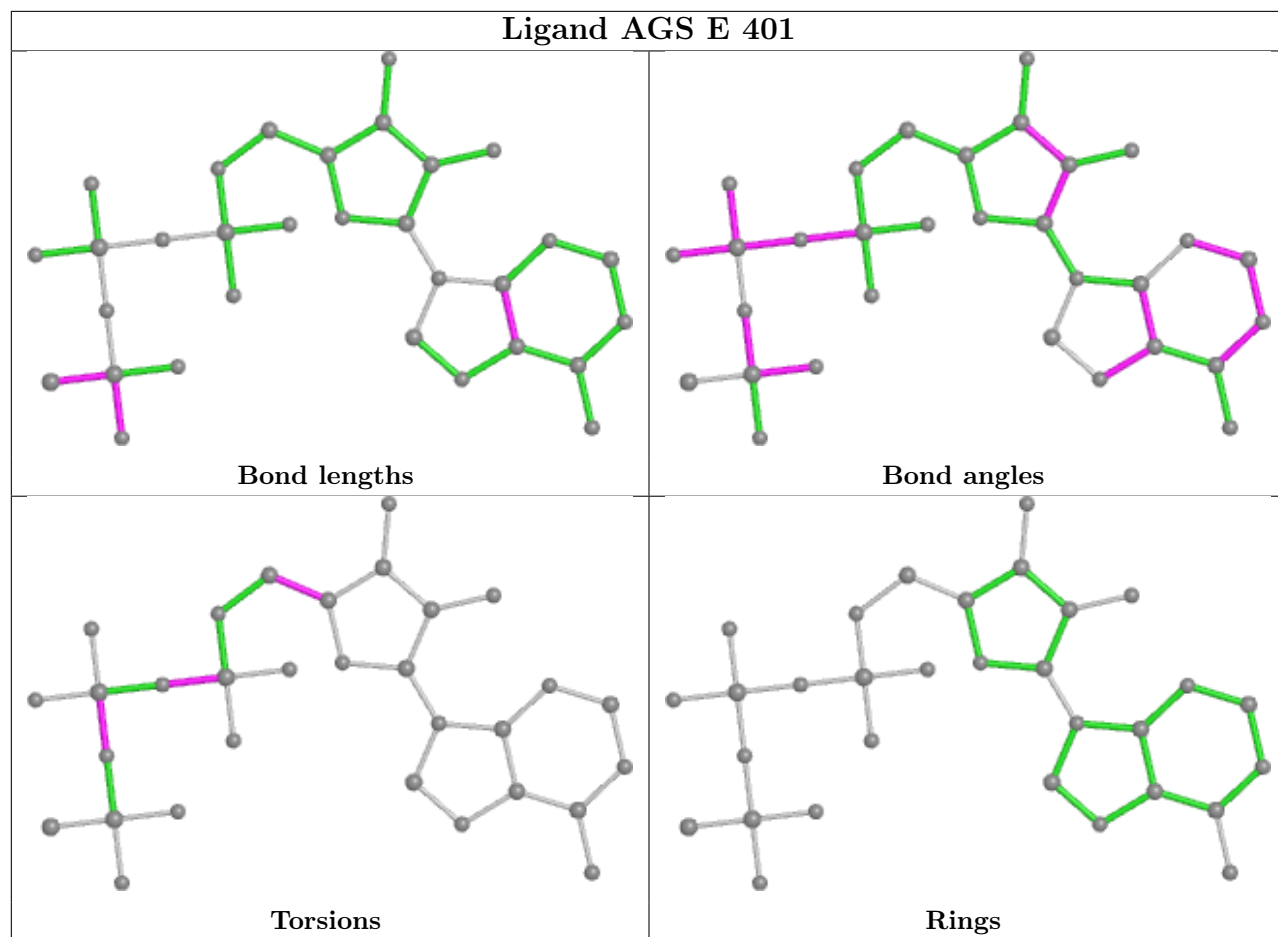


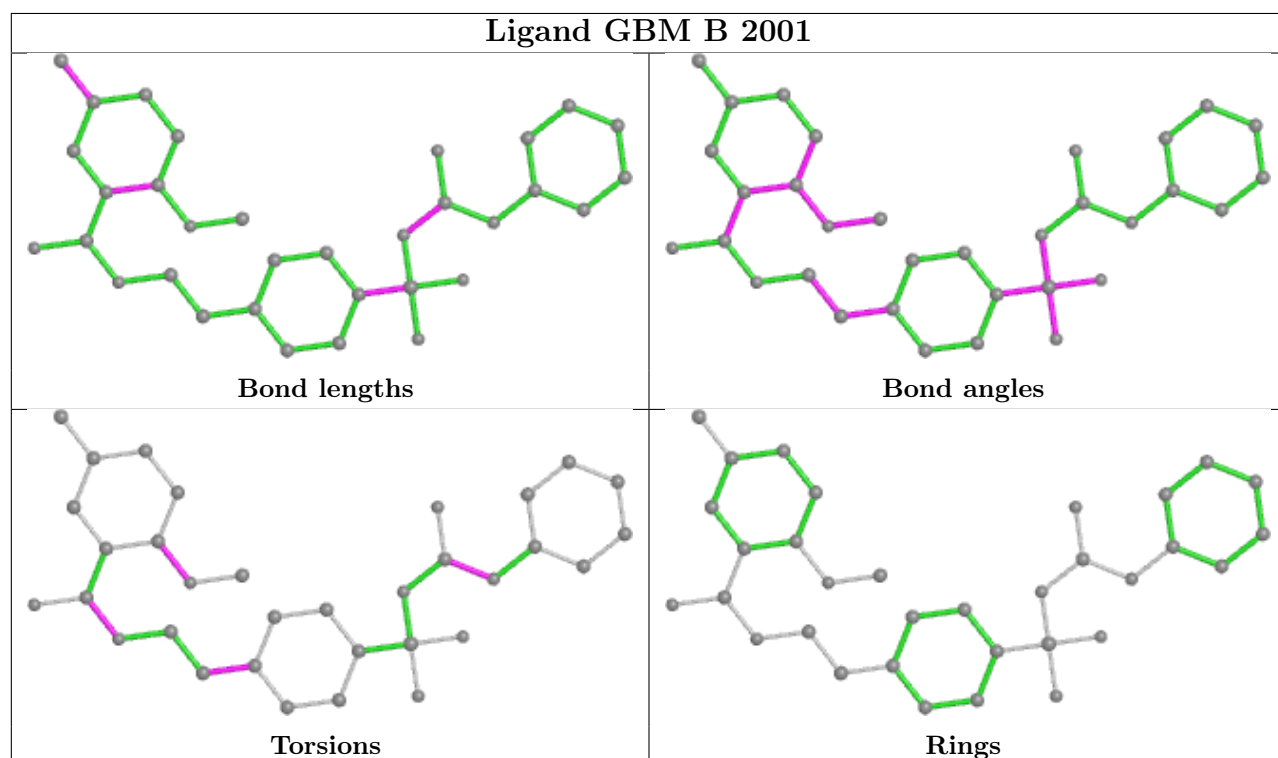
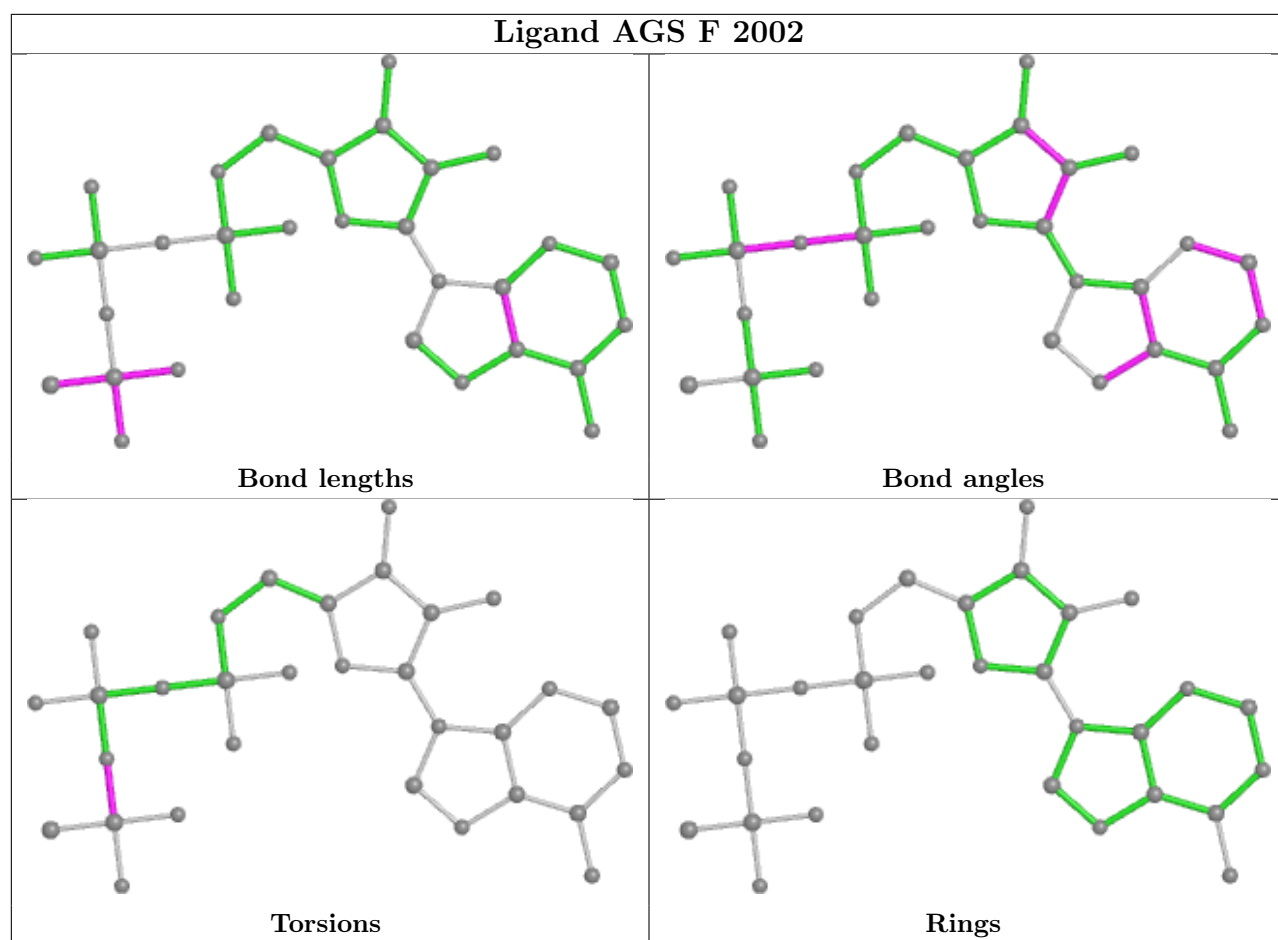






Ligand AGS E 401





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.

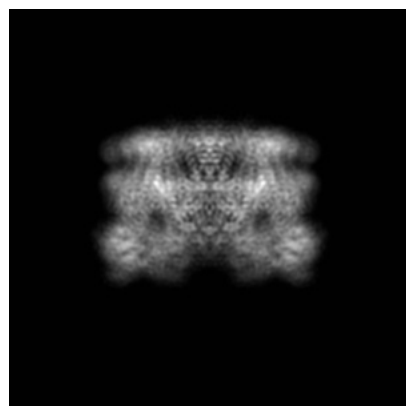
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6832. These allow visual inspection of the internal detail of the map and identification of artifacts.

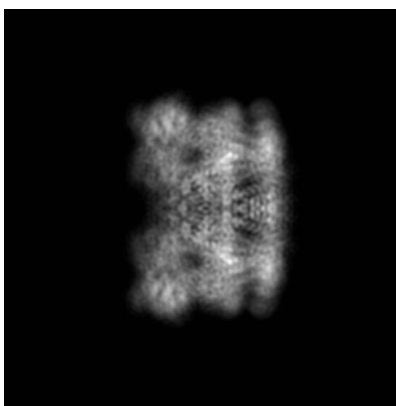
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

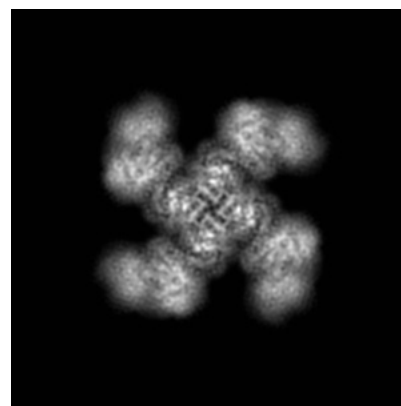
6.1.1 Primary map



X

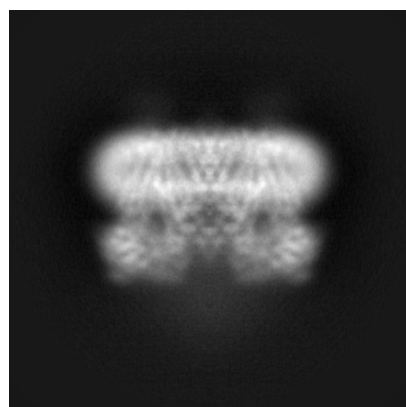


Y

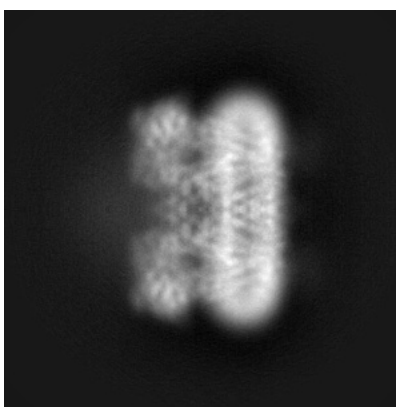


Z

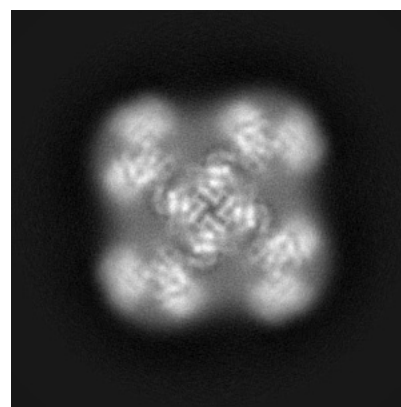
6.1.2 Raw map



X



Y

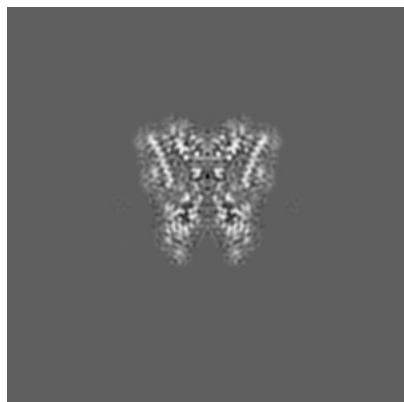


Z

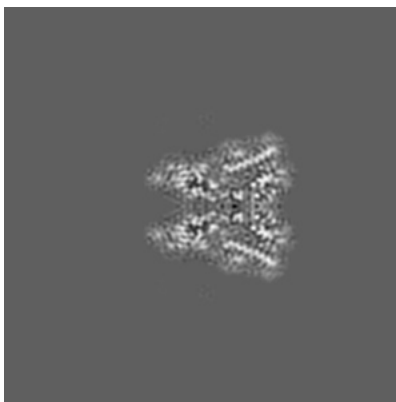
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

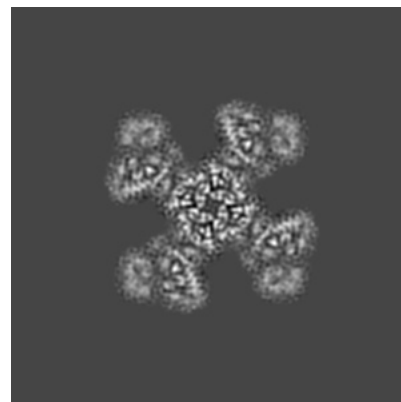
6.2.1 Primary map



X Index: 156

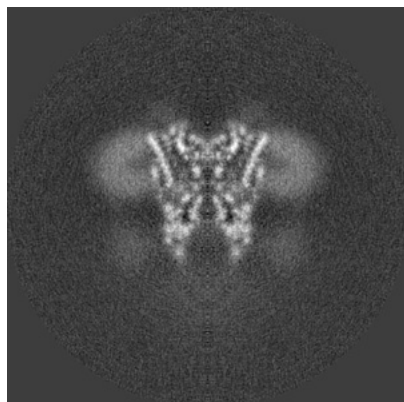


Y Index: 156

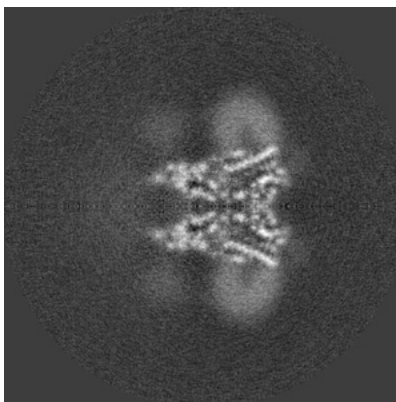


Z Index: 156

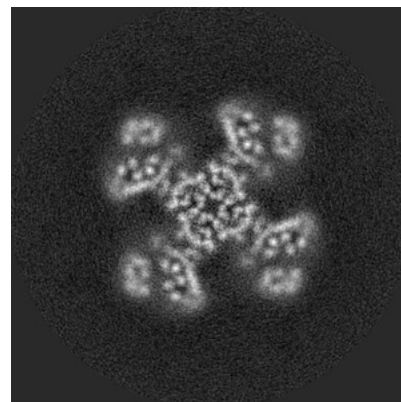
6.2.2 Raw map



X Index: 156



Y Index: 156

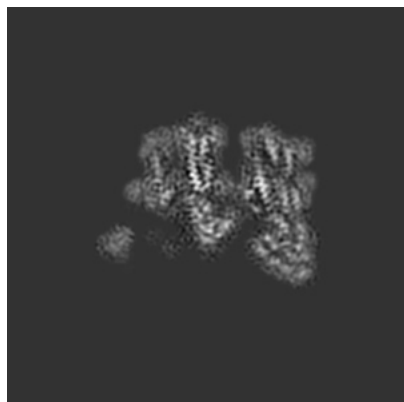


Z Index: 156

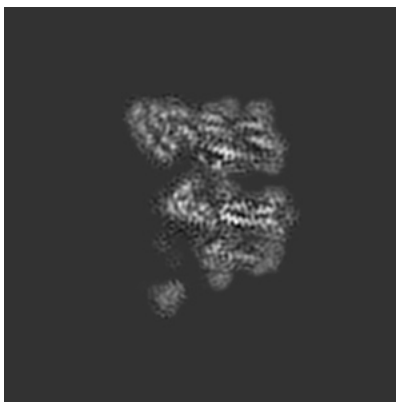
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

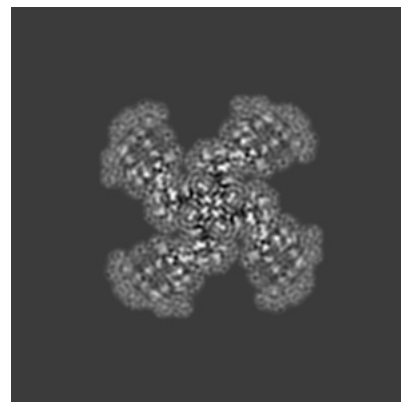
6.3.1 Primary map



X Index: 187

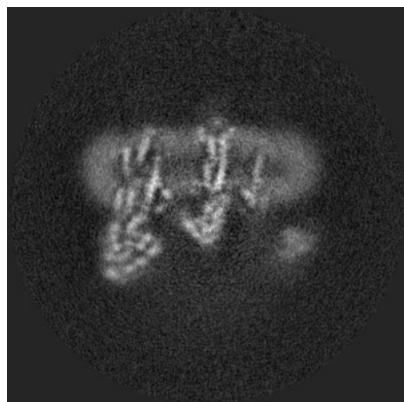


Y Index: 125

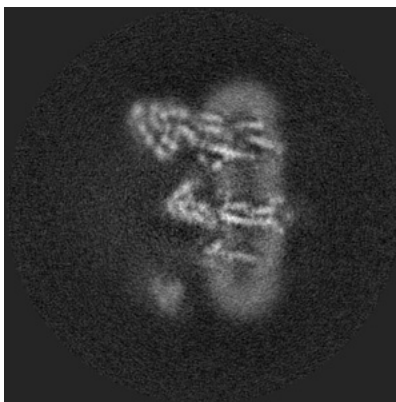


Z Index: 175

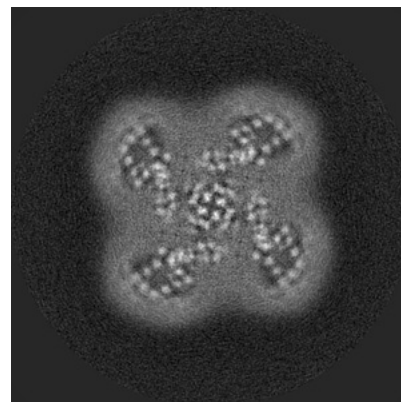
6.3.2 Raw map



X Index: 125



Y Index: 125

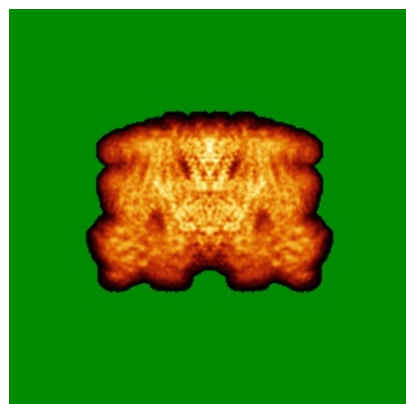


Z Index: 173

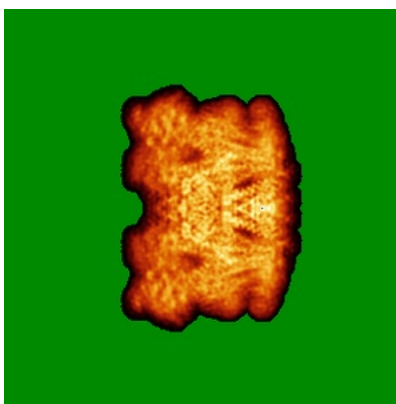
The images above show the largest variance slices of the map in three orthogonal directions.

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

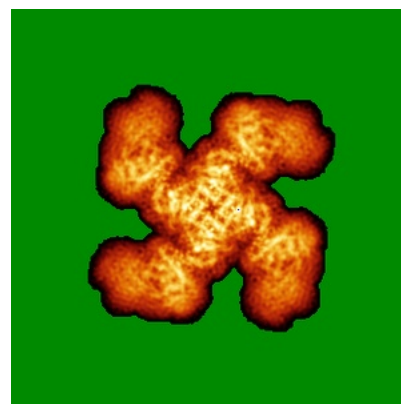
6.4.1 Primary map



X

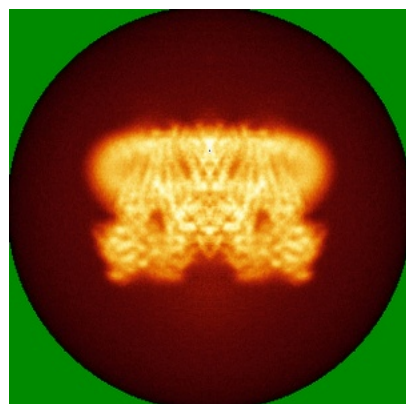


Y

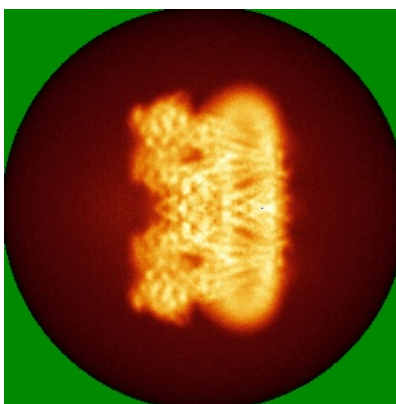


Z

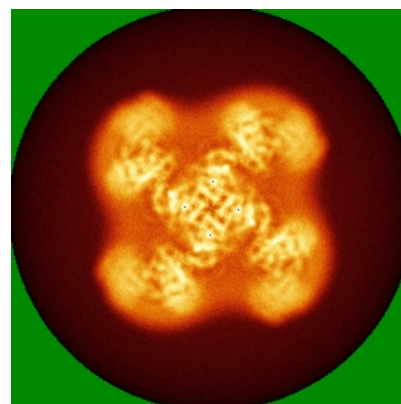
6.4.2 Raw map



X



Y

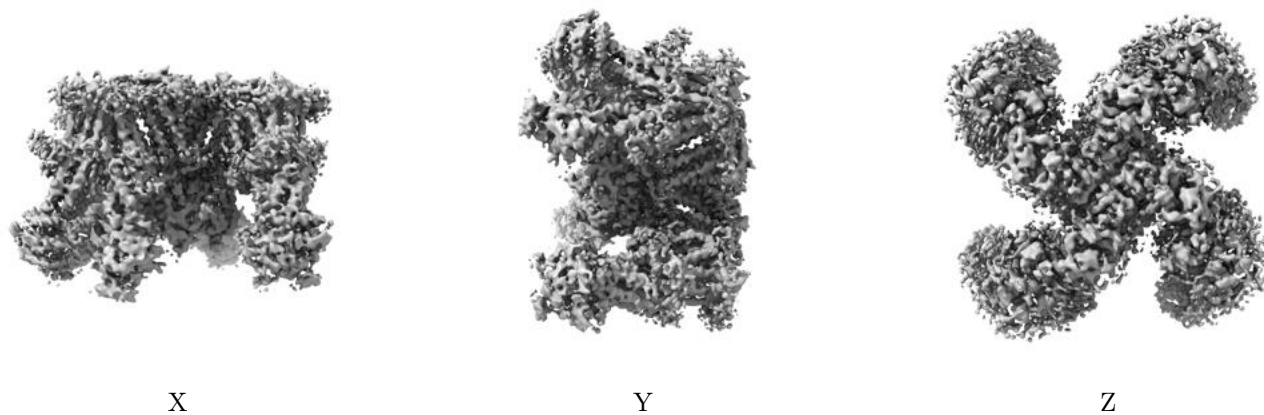


Z

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.

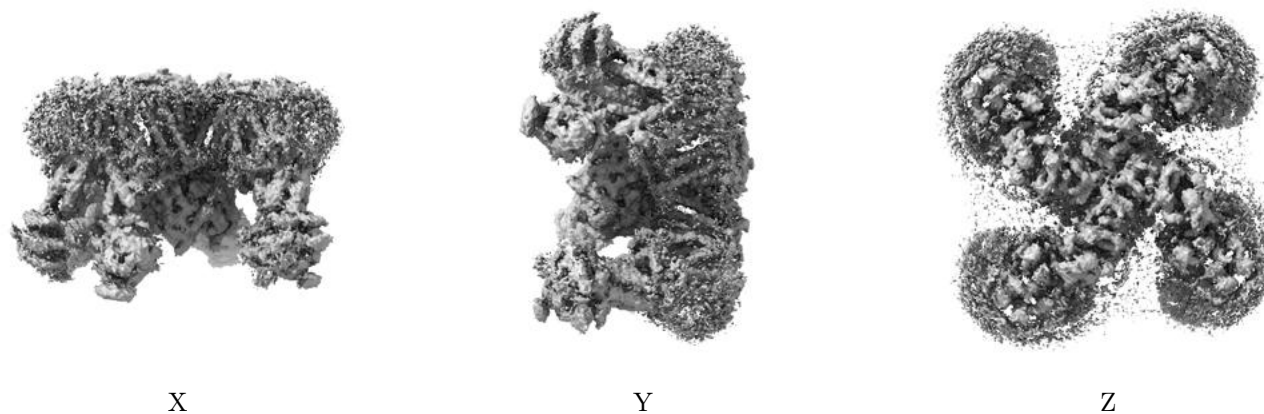
6.5 Orthogonal surface views [i](#)

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.

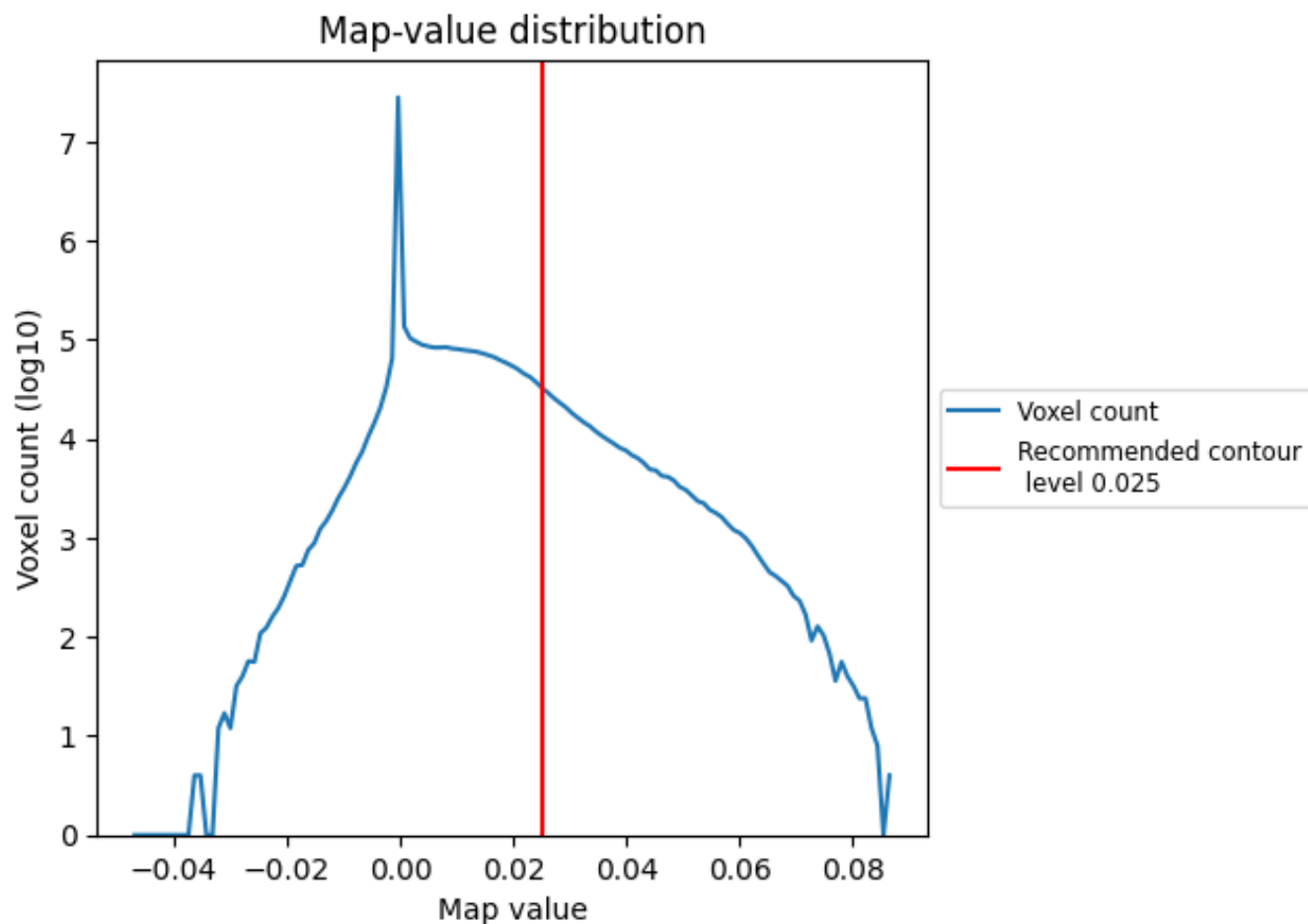
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

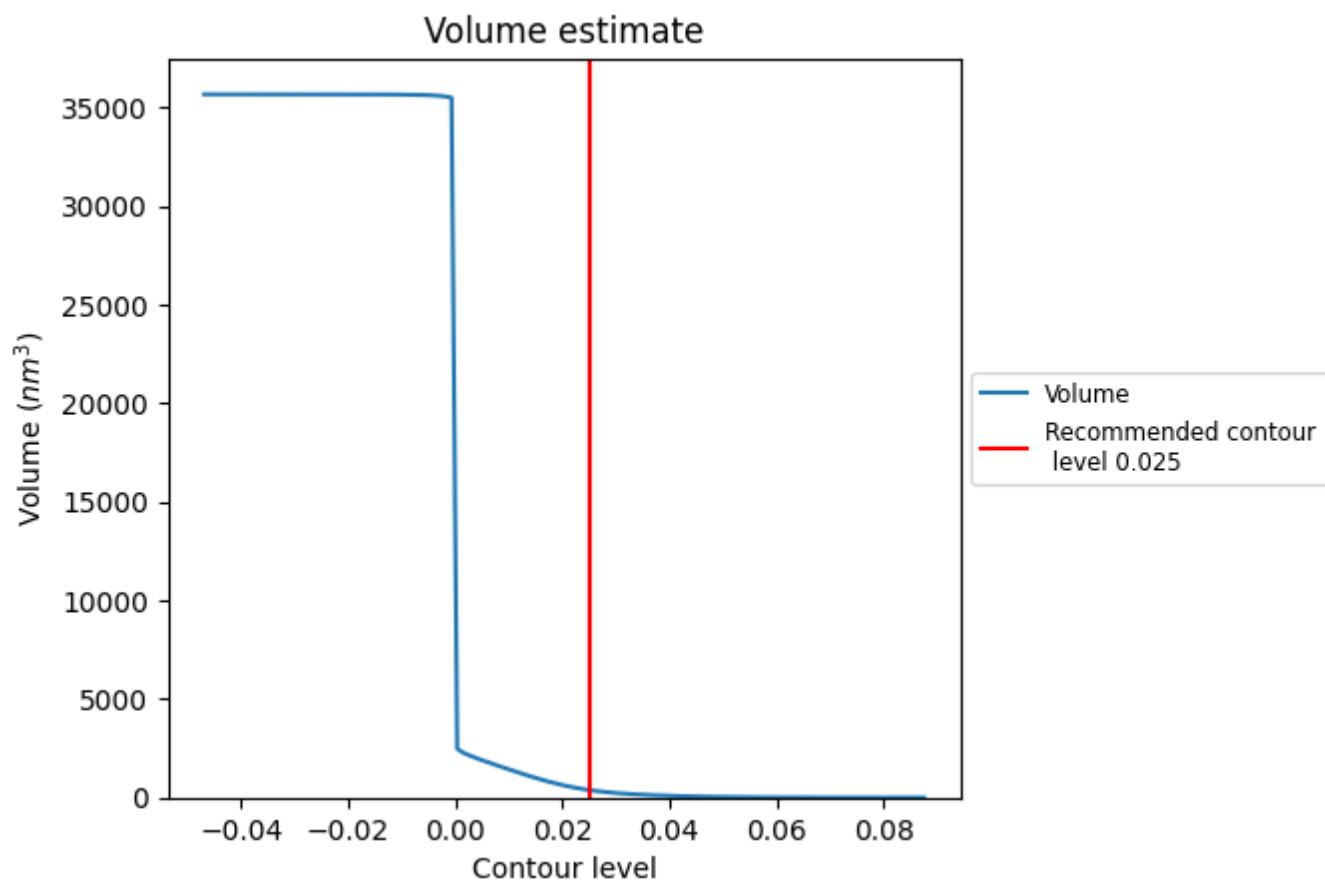
This section contains the results of statistical analysis of the map.

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.

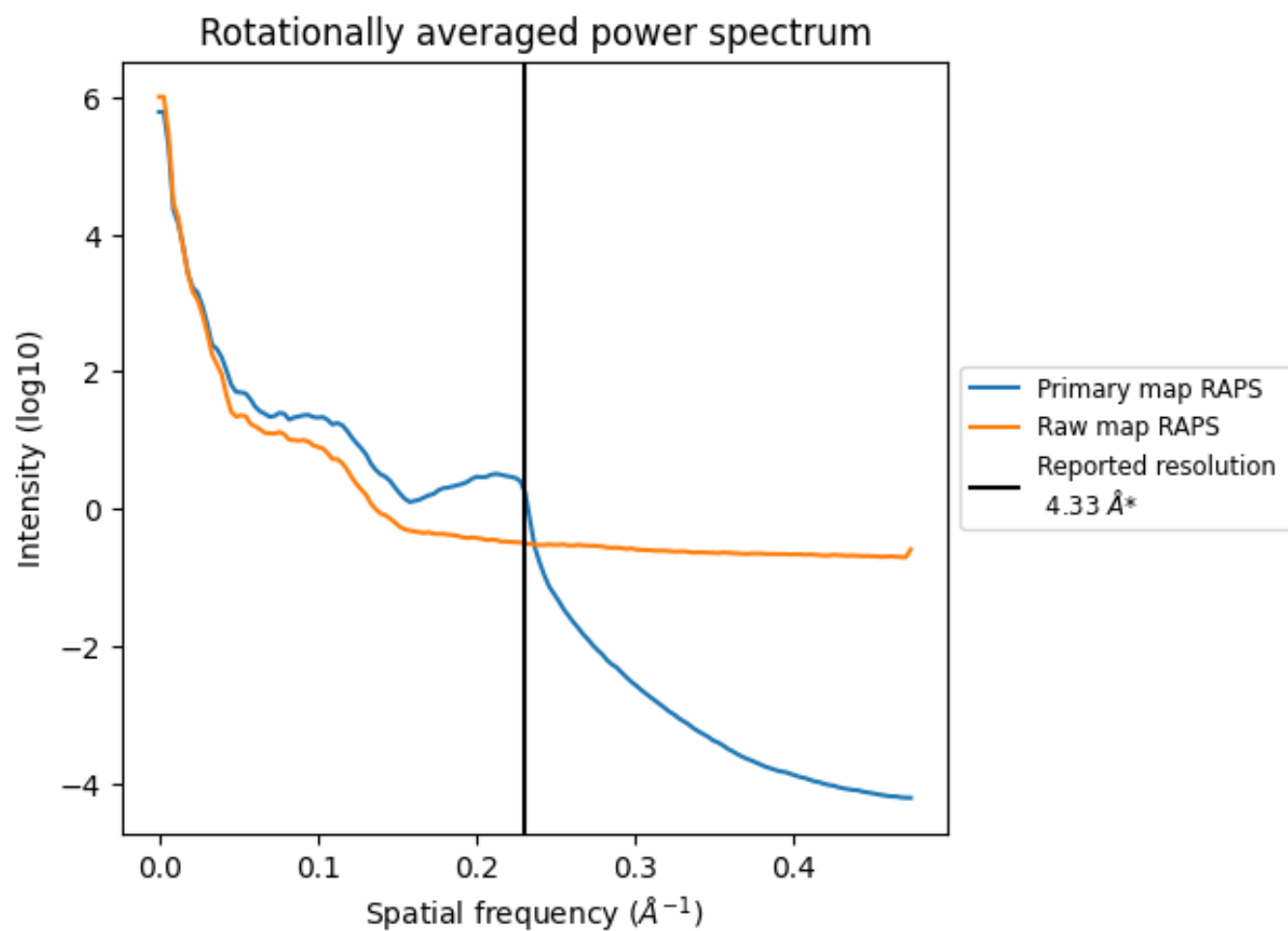
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 382 nm³; this corresponds to an approximate mass of 345 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 ⓘ

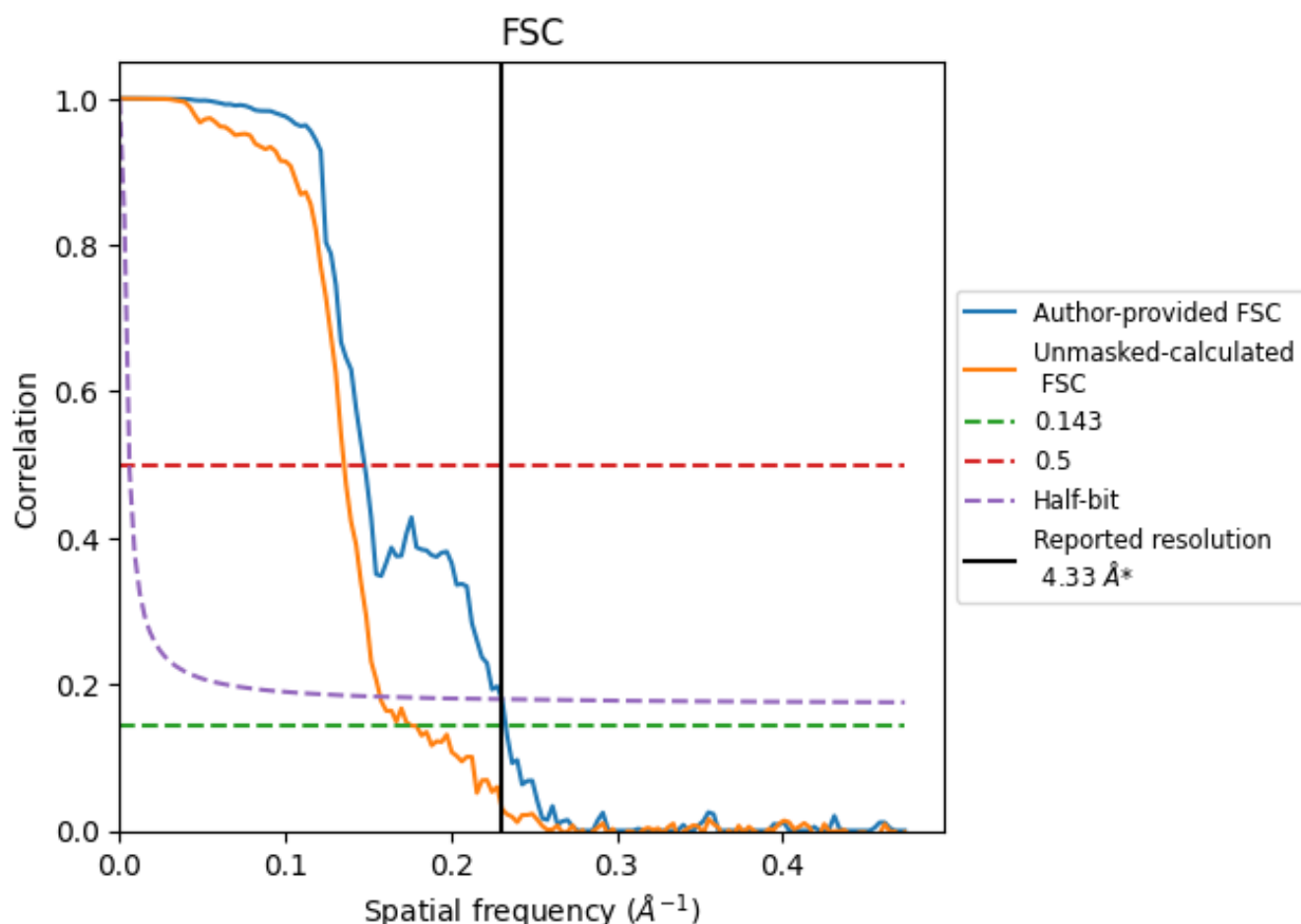


*Reported resolution corresponds to spatial frequency of 0.231 \AA^{-1}

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 0.231 Å⁻¹

8.2 Resolution estimates [i](#)

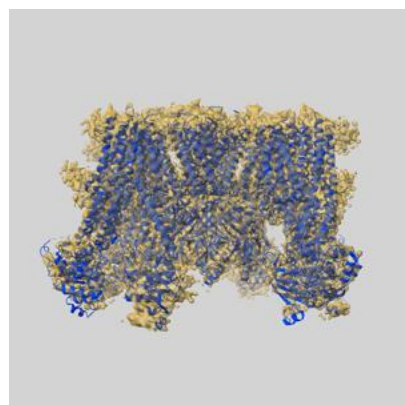
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.33	-	-
Author-provided FSC curve	4.29	6.77	4.33
Unmasked-calculated*	5.58	7.38	6.35

*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 5.58 differs from the reported value 4.33 by more than 10 %

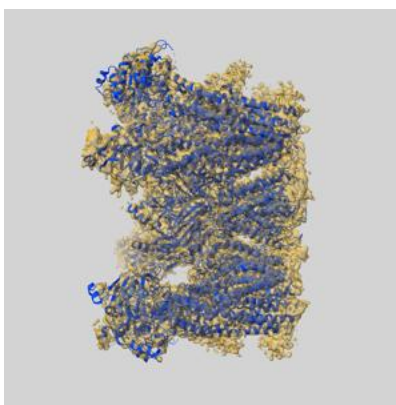
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6832 and PDB model 5YKF. Per-residue inclusion information can be found in section [3](#) on page [6](#).

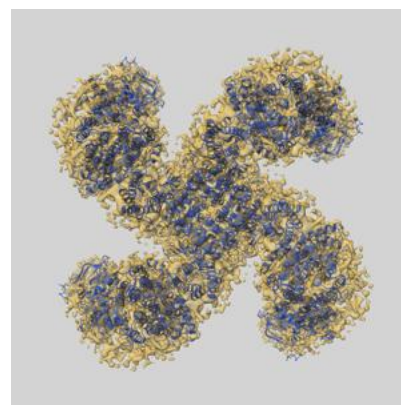
9.1 Map-model overlay [i](#)



X



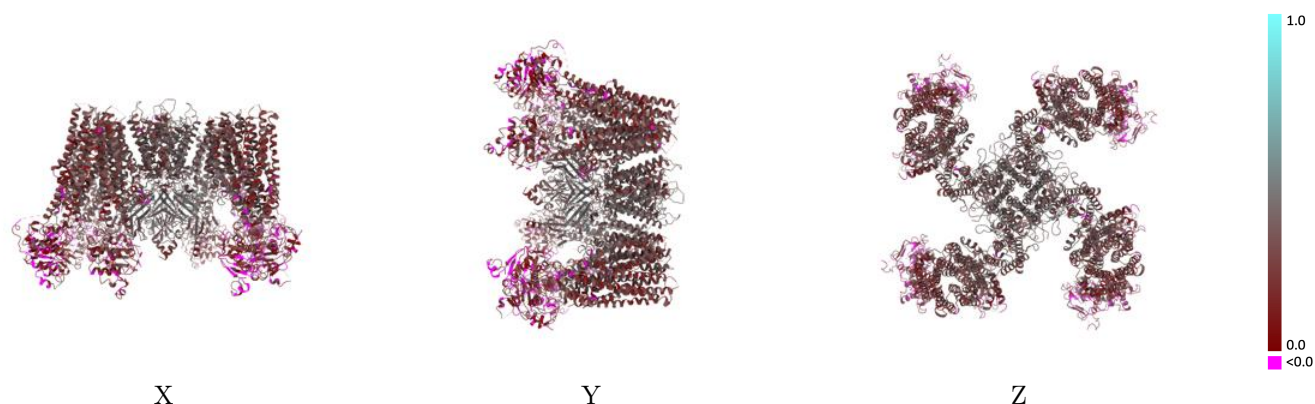
Y



Z

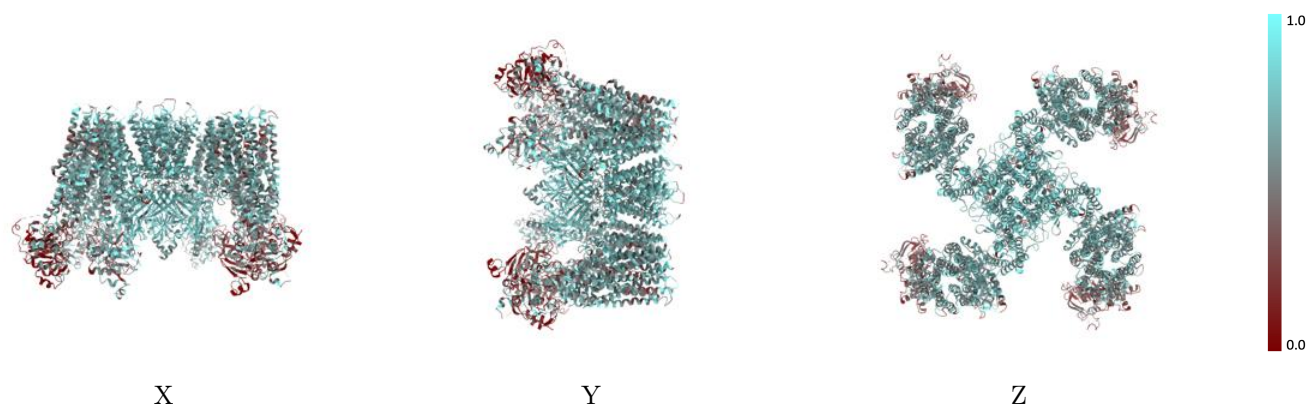
The images above show the 3D surface view of the map at the recommended contour level 0.025 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



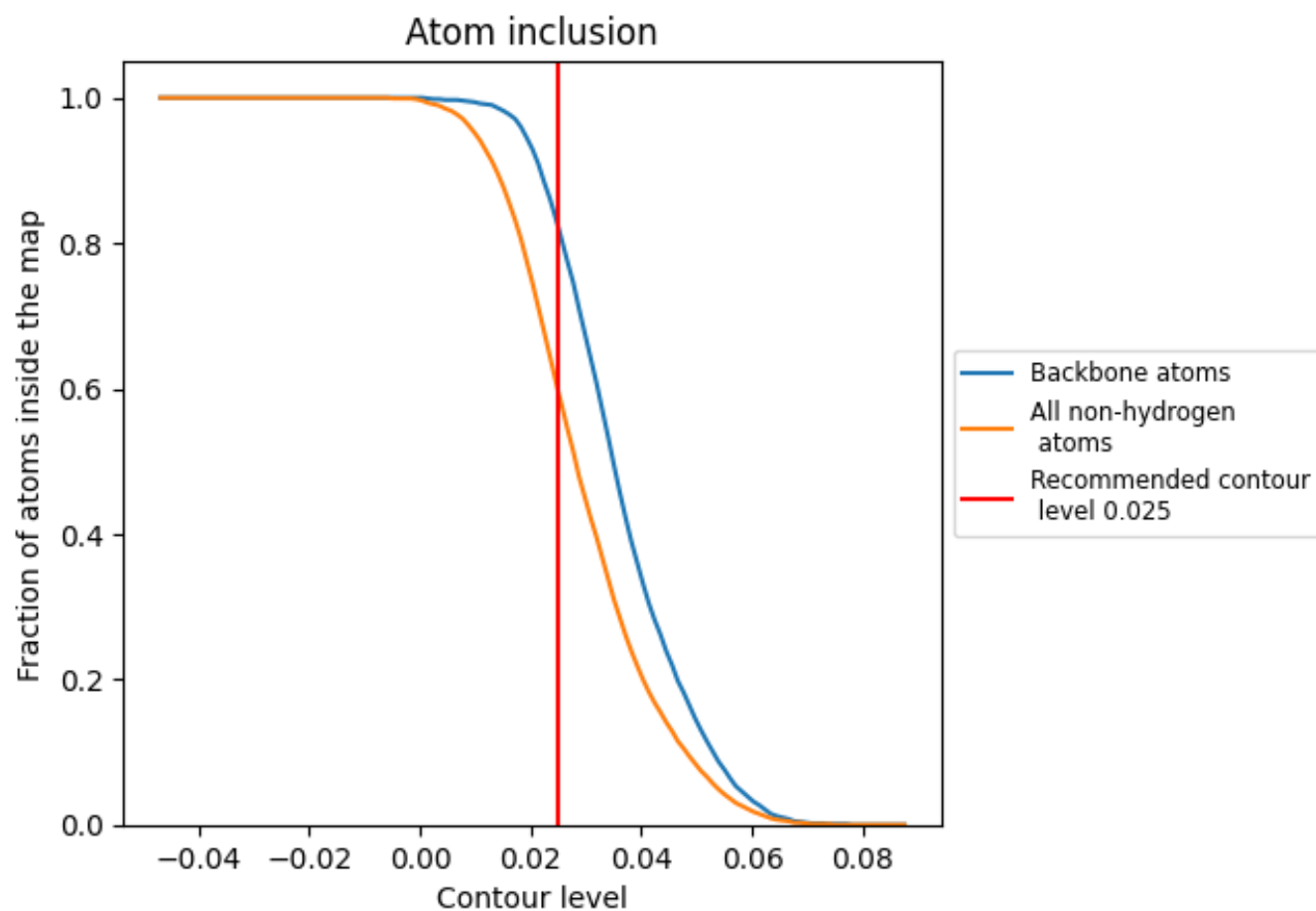
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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



At the recommended contour level, 82% of all backbone atoms, 60% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.025) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5950	<div></div> 0.2740
A	<div></div> 0.7660	<div></div> 0.3990
B	<div></div> 0.5540	<div></div> 0.2420
C	<div></div> 0.7640	<div></div> 0.3970
D	<div></div> 0.5540	<div></div> 0.2430
E	<div></div> 0.7640	<div></div> 0.3990
F	<div></div> 0.5540	<div></div> 0.2440
G	<div></div> 0.7610	<div></div> 0.4000
H	<div></div> 0.5540	<div></div> 0.2430

1.0

0.0

<0.0