wwPDB EM Validation Summary Report (i)

Nov 18, 2023 – 06:17 am GMT

PDB ID	:	8GW6
EMDB ID	:	EMD-34303
Title	:	AtSLAC1 6D mutant in closed state
Authors	:	Lee, Y.; Lee, S.
Deposited on	:	2022-09-16
Resolution	:	3.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references (i)) were used in the production of this report:

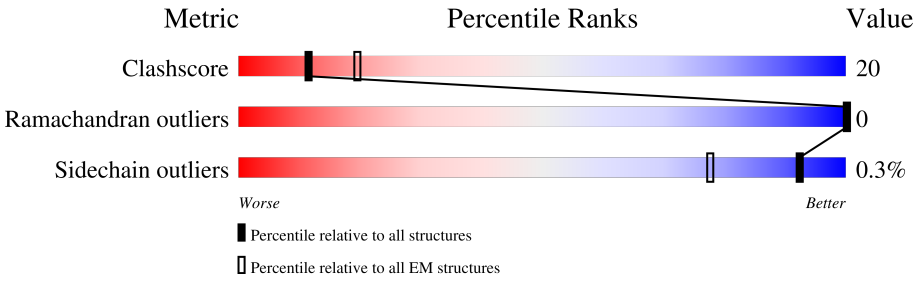
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	826	28% 16% 56%
1	B	826	29% 16% 56%
1	C	826	29% 16% 56%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 9030 atoms, of which 147 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 Guard cell S-type anion channel SLAC1,Green fluorescent protein (Fragment).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	367	Total	C	N	O	S	1	0
			2925	1975	460	475	15		
1	B	367	Total	C	N	O	S	1	0
			2925	1975	460	475	15		
1	C	367	Total	C	N	O	S	1	0
			2925	1975	460	475	15		

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	62	ASP	THR	engineered mutation	UNP Q9LD83
A	65	ASP	SER	engineered mutation	UNP Q9LD83
A	107	ASP	SER	engineered mutation	UNP Q9LD83
A	124	ASP	SER	engineered mutation	UNP Q9LD83
A	146	ASP	SER	engineered mutation	UNP Q9LD83
A	152	ASP	SER	conflict	UNP Q9LD83
A	557	GLY	-	linker	UNP Q9LD83
A	558	SER	-	linker	UNP Q9LD83
A	559	GLU	-	linker	UNP Q9LD83
A	560	ASN	-	linker	UNP Q9LD83
A	561	LEU	-	linker	UNP Q9LD83
A	562	TYR	-	linker	UNP Q9LD83
A	563	PHE	-	linker	UNP Q9LD83
A	564	GLN	-	linker	UNP Q9LD83
A	565	SER	-	linker	UNP Q9LD83
A	567	SER	ARG	conflict	UNP A0A059PIQ0
A	595	ARG	SER	conflict	UNP A0A059PIQ0
A	637	SER	ALA	conflict	UNP A0A059PIQ0
A	645	ARG	GLN	conflict	UNP A0A059PIQ0
A	771	VAL	ALA	conflict	UNP A0A059PIQ0
A	804	TYR	ARG	conflict	UNP A0A059PIQ0
A	806	TYR	-	expression tag	UNP A0A059PIQ0
A	807	ASP	-	expression tag	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
A	808	VAL	-	expression tag	UNP A0A059PIQ0
A	809	PRO	-	expression tag	UNP A0A059PIQ0
A	810	ASP	-	expression tag	UNP A0A059PIQ0
A	811	TYR	-	expression tag	UNP A0A059PIQ0
A	812	ALA	-	expression tag	UNP A0A059PIQ0
A	813	GLY	-	expression tag	UNP A0A059PIQ0
A	814	GLY	-	expression tag	UNP A0A059PIQ0
A	815	GLY	-	expression tag	UNP A0A059PIQ0
A	816	SER	-	expression tag	UNP A0A059PIQ0
A	817	HIS	-	expression tag	UNP A0A059PIQ0
A	818	HIS	-	expression tag	UNP A0A059PIQ0
A	819	HIS	-	expression tag	UNP A0A059PIQ0
A	820	HIS	-	expression tag	UNP A0A059PIQ0
A	821	HIS	-	expression tag	UNP A0A059PIQ0
A	822	HIS	-	expression tag	UNP A0A059PIQ0
A	823	HIS	-	expression tag	UNP A0A059PIQ0
A	824	HIS	-	expression tag	UNP A0A059PIQ0
A	825	HIS	-	expression tag	UNP A0A059PIQ0
A	826	HIS	-	expression tag	UNP A0A059PIQ0
B	62	ASP	THR	engineered mutation	UNP Q9LD83
B	65	ASP	SER	engineered mutation	UNP Q9LD83
B	107	ASP	SER	engineered mutation	UNP Q9LD83
B	124	ASP	SER	engineered mutation	UNP Q9LD83
B	146	ASP	SER	engineered mutation	UNP Q9LD83
B	152	ASP	SER	conflict	UNP Q9LD83
B	557	GLY	-	linker	UNP Q9LD83
B	558	SER	-	linker	UNP Q9LD83
B	559	GLU	-	linker	UNP Q9LD83
B	560	ASN	-	linker	UNP Q9LD83
B	561	LEU	-	linker	UNP Q9LD83
B	562	TYR	-	linker	UNP Q9LD83
B	563	PHE	-	linker	UNP Q9LD83
B	564	GLN	-	linker	UNP Q9LD83
B	565	SER	-	linker	UNP Q9LD83
B	567	SER	ARG	conflict	UNP A0A059PIQ0
B	595	ARG	SER	conflict	UNP A0A059PIQ0
B	637	SER	ALA	conflict	UNP A0A059PIQ0
B	645	ARG	GLN	conflict	UNP A0A059PIQ0
B	771	VAL	ALA	conflict	UNP A0A059PIQ0
B	804	TYR	ARG	conflict	UNP A0A059PIQ0
B	806	TYR	-	expression tag	UNP A0A059PIQ0
B	807	ASP	-	expression tag	UNP A0A059PIQ0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	808	VAL	-	expression tag	UNP A0A059PIQ0
B	809	PRO	-	expression tag	UNP A0A059PIQ0
B	810	ASP	-	expression tag	UNP A0A059PIQ0
B	811	TYR	-	expression tag	UNP A0A059PIQ0
B	812	ALA	-	expression tag	UNP A0A059PIQ0
B	813	GLY	-	expression tag	UNP A0A059PIQ0
B	814	GLY	-	expression tag	UNP A0A059PIQ0
B	815	GLY	-	expression tag	UNP A0A059PIQ0
B	816	SER	-	expression tag	UNP A0A059PIQ0
B	817	HIS	-	expression tag	UNP A0A059PIQ0
B	818	HIS	-	expression tag	UNP A0A059PIQ0
B	819	HIS	-	expression tag	UNP A0A059PIQ0
B	820	HIS	-	expression tag	UNP A0A059PIQ0
B	821	HIS	-	expression tag	UNP A0A059PIQ0
B	822	HIS	-	expression tag	UNP A0A059PIQ0
B	823	HIS	-	expression tag	UNP A0A059PIQ0
B	824	HIS	-	expression tag	UNP A0A059PIQ0
B	825	HIS	-	expression tag	UNP A0A059PIQ0
B	826	HIS	-	expression tag	UNP A0A059PIQ0
C	62	ASP	THR	engineered mutation	UNP Q9LD83
C	65	ASP	SER	engineered mutation	UNP Q9LD83
C	107	ASP	SER	engineered mutation	UNP Q9LD83
C	124	ASP	SER	engineered mutation	UNP Q9LD83
C	146	ASP	SER	engineered mutation	UNP Q9LD83
C	152	ASP	SER	conflict	UNP Q9LD83
C	557	GLY	-	linker	UNP Q9LD83
C	558	SER	-	linker	UNP Q9LD83
C	559	GLU	-	linker	UNP Q9LD83
C	560	ASN	-	linker	UNP Q9LD83
C	561	LEU	-	linker	UNP Q9LD83
C	562	TYR	-	linker	UNP Q9LD83
C	563	PHE	-	linker	UNP Q9LD83
C	564	GLN	-	linker	UNP Q9LD83
C	565	SER	-	linker	UNP Q9LD83
C	567	SER	ARG	conflict	UNP A0A059PIQ0
C	595	ARG	SER	conflict	UNP A0A059PIQ0
C	637	SER	ALA	conflict	UNP A0A059PIQ0
C	645	ARG	GLN	conflict	UNP A0A059PIQ0
C	771	VAL	ALA	conflict	UNP A0A059PIQ0
C	804	TYR	ARG	conflict	UNP A0A059PIQ0
C	806	TYR	-	expression tag	UNP A0A059PIQ0
C	807	ASP	-	expression tag	UNP A0A059PIQ0

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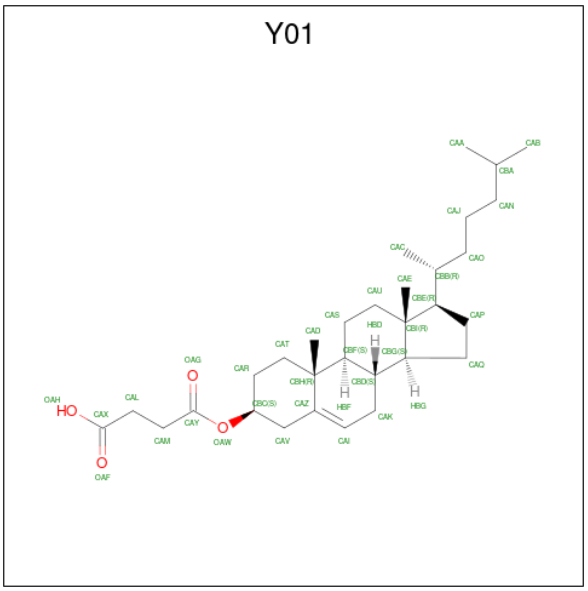
Chain	Residue	Modelled	Actual	Comment	Reference
C	808	VAL	-	expression tag	UNP A0A059PIQ0
C	809	PRO	-	expression tag	UNP A0A059PIQ0
C	810	ASP	-	expression tag	UNP A0A059PIQ0
C	811	TYR	-	expression tag	UNP A0A059PIQ0
C	812	ALA	-	expression tag	UNP A0A059PIQ0
C	813	GLY	-	expression tag	UNP A0A059PIQ0
C	814	GLY	-	expression tag	UNP A0A059PIQ0
C	815	GLY	-	expression tag	UNP A0A059PIQ0
C	816	SER	-	expression tag	UNP A0A059PIQ0
C	817	HIS	-	expression tag	UNP A0A059PIQ0
C	818	HIS	-	expression tag	UNP A0A059PIQ0
C	819	HIS	-	expression tag	UNP A0A059PIQ0
C	820	HIS	-	expression tag	UNP A0A059PIQ0
C	821	HIS	-	expression tag	UNP A0A059PIQ0
C	822	HIS	-	expression tag	UNP A0A059PIQ0
C	823	HIS	-	expression tag	UNP A0A059PIQ0
C	824	HIS	-	expression tag	UNP A0A059PIQ0
C	825	HIS	-	expression tag	UNP A0A059PIQ0
C	826	HIS	-	expression tag	UNP A0A059PIQ0

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	AltConf
2	A	1	Total Cl 1 1	0
2	B	1	Total Cl 1 1	0
2	C	1	Total Cl 1 1	0

- Molecule 3 is CHOLESTEROL HEMISUCCINATE (three-letter code: Y01) (formula: $C_{31}H_{50}O_4$).



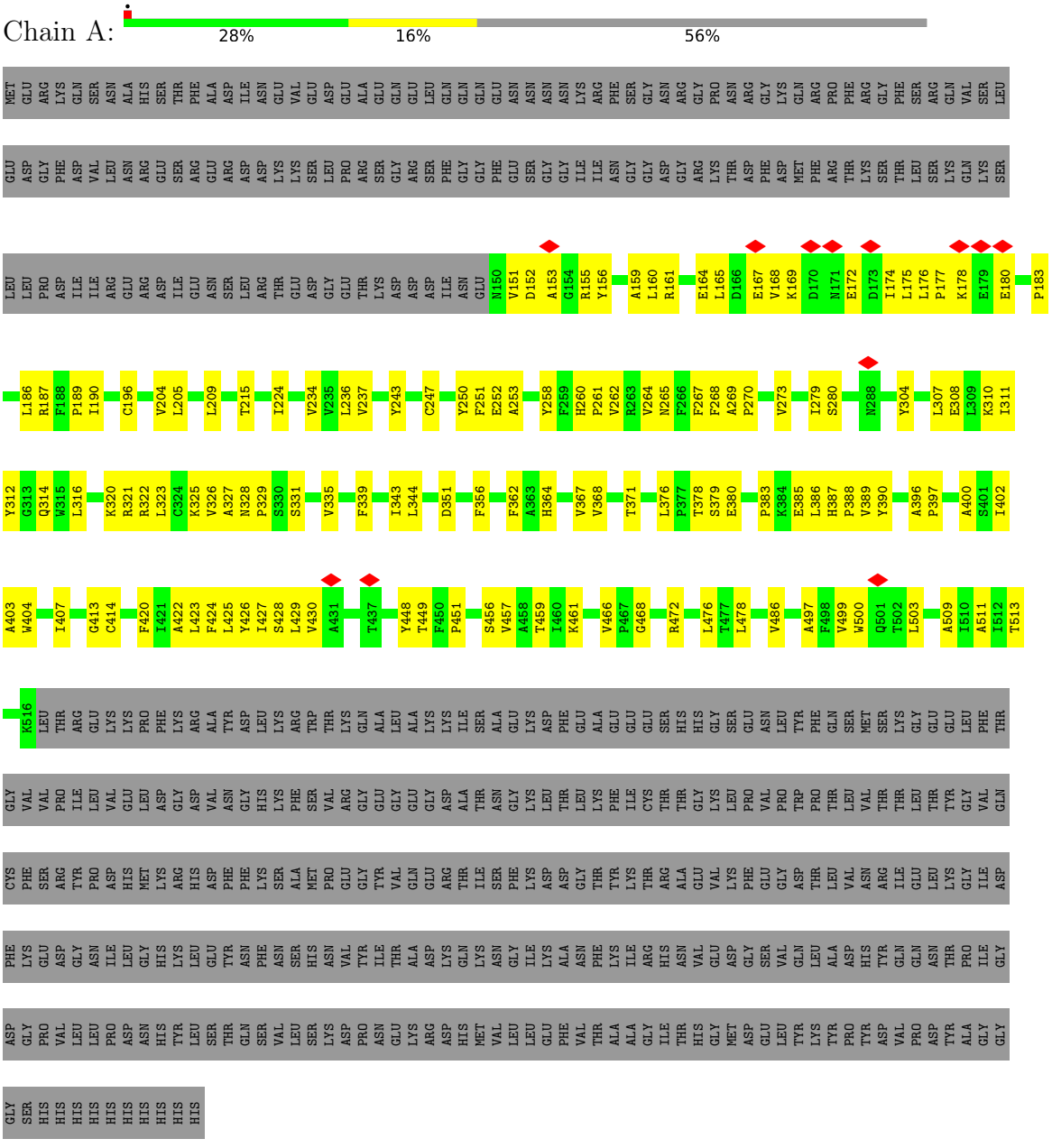
Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	H	O	0
			84	31	49	4	
3	A	1	Total	C	H	O	0
			84	31	49	4	
3	C	1	Total	C	H	O	0
			84	31	49	4	

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.

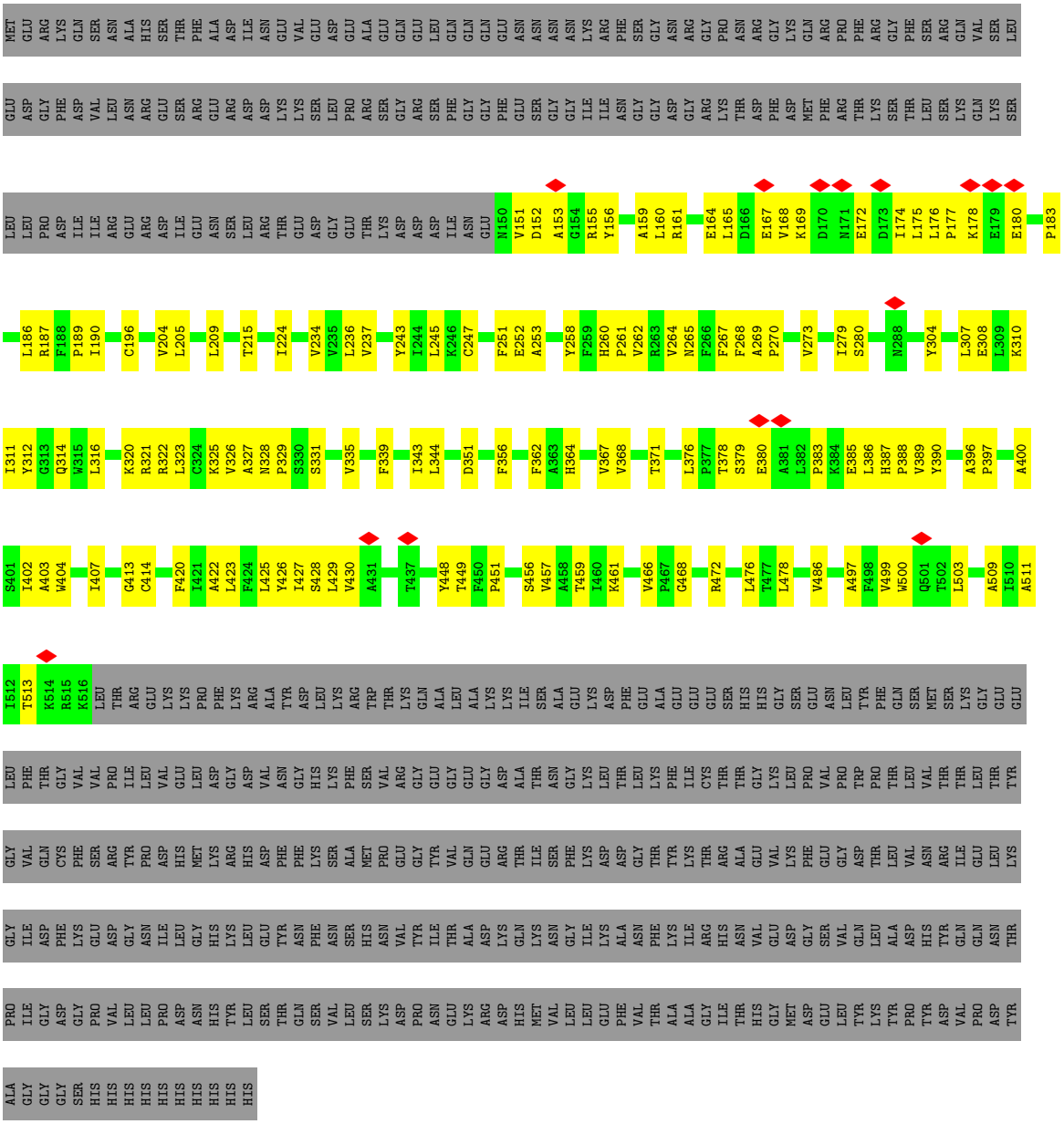
• Molecule 1: Guard cell S-type anion channel SLAC1,Green fluorescent protein (Fragment)

Chain A:



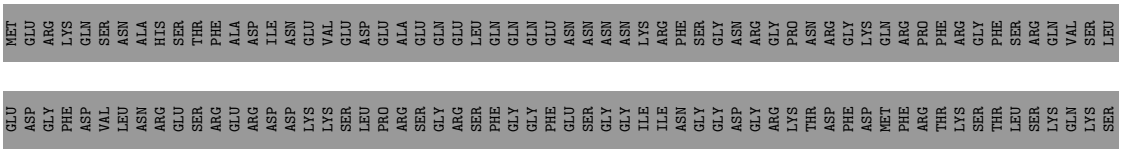
• Molecule 1: Guard cell S-type anion channel SLAC1,Green fluorescent protein (Fragment)

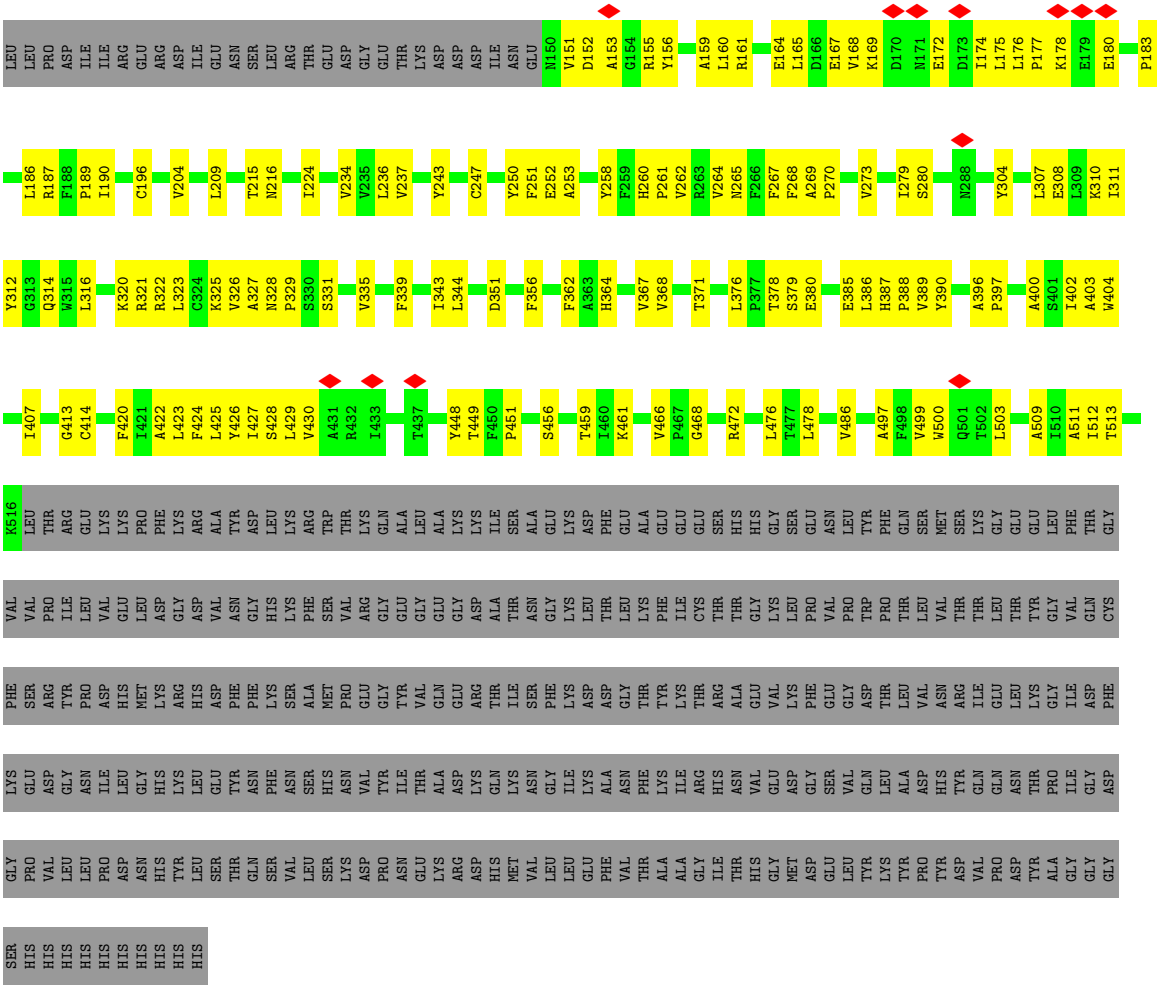
Chain B:



• Molecule 1: Guard cell S-type anion channel SLAC1,Green fluorescent protein (Fragment)

Chain C:




LEU LEU PRO ASP ILE ILE ARG GLU ARG ASP ILE GLU ASN SER LEU ARG THR GLU ASP GLY GLU THR LYS ASP ASP ILE ASN GLU
N150 V151 D152 A153 G154 R155 Y156 A159 L160 R161 E164 L165 D166 E167 V168 K169 D170 N171 E172 D173 I174 L175 L176 P177 K178 E179 E180 P183
L186 R187 F188 P189 I190 C196 V204 L209 T215 N216 I224 V234 V235 L236 V237 Y243 C247 Y250 F251 E252 A253 Y258 F259 H260 P261 V262 R263 V264 N265 F266 F267 F268 A269 P270 V273 I279 S280 N288 Y304 L307 E308 L309 K310 I311
Y312 G313 Q314 W315 L316 K320 R321 R322 L323 C324 K325 V326 A327 N328 P329 S330 S331 V335 F339 I343 L344 D351 F356 F362 A363 H364 V367 V368 T371 L376 P377 T378 S379 E380 E385 L386 H387 P388 V389 Y390 A396 P397 A400 S401 I402 A403 W404
I407 G413 C414 F420 I421 A422 L423 F424 L425 Y426 I427 S428 L429 V430 A431 R432 I433 T437 Y448 T449 F450 P451 S456 T459 I460 K461 V466 P467 G468 R472 L476 T477 L478 V486 A497 F498 V499 W500 Q501 T502 L503 A509 I510 A511 I512 T513
K516 LEU THR ARG GLU LYS LYS PRO PHE LYS ARG ALA TYR ASP LEU LYS ARG TRP THR LYS GLN ALA LEU ALA LYS LYS ILE SER ALA GLU LYS ASP PHE GLU LEU ALA GLU GLU GLU SER HIS HIS GLY SER GLU ASN LEU TYR PHE GLN SER MET SER LYS GLY GLU GLU LEU PHE THR GLY
VAL VAL PRO ILE LEU VAL GLU LEU ASP GLY ASP VAL ASN GLY HIS LYS PHE SER VAL ARG GLY GLU GLU GLY GLY ASP ALA THR ASN GLY LYS LEU THR LEU LYS PHE ILE CYS THR THR GLY LYS LEU PRO VAL PRO TRP PRO THR LEU VAL THR THR LEU THR TYR GLY VAL THR LEU
PHE SER ARG TYR PRO ASP HIS MET LYS ARG HIS ASP PHE PHE LYS SER ALA MET PRO GLU GLY TYR VAL GLN GLU ARG THR ILE SER PHE LYS ASP ASP GLY THR TYR LYS THR ARG ALA GLU VAL LYS PHE GLU GLY ASP THR LEU VAL ASN ARG ILE GLU LEU LYS GLY ILE ASP PHE
LYS GLU ASP GLY ASN ILE LEU GLY HIS LYS LEU GLU TYR ASN PHE ASN SER HIS ASN VAL TYR ILE THR ALA ASP LYS GLN LYS SER ASN GLY ILE LYS ALA ASN PHE LYS ILE ARG HIS ASN VAL GLU ASP GLY SER VAL GLN LEU ALA ASP HIS TYR GLN GLN ASN THR PRO ILE GLY ASP
GLY PRO VAL LEU LEU PRO ASP ASN HIS TYR LEU SER THR GLN SER VAL LEU SER LYS ASP PRO ASN GLU LYS ARG ASP HIS MET VAL LEU LEU GLU PHE VAL THR ALA ALA GLY ILE THR HIS GLY MET ASP GLU LEU TYR LYS TYR PRO TYR ASP VAL PRO ASP TYR ALA GLY GLY GLY
SER HIS HIS HIS HIS HIS HIS HIS HIS HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C3	Depositor
Number of particles used	69390	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	700	Depositor
Maximum defocus (nm)	1900	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.560	Depositor
Minimum map value	-1.103	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.049	Depositor
Recommended contour level	0.176	Depositor
Map size (Å)	204.0, 204.0, 204.0	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.85, 0.85, 0.85	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, Y01

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	0.25	0/3031	0.40	0/4144
1	B	0.25	0/3031	0.40	0/4144
1	C	0.25	0/3031	0.41	0/4144
All	All	0.25	0/9093	0.40	0/12432

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	2925	0	2940	116	0
1	B	2925	0	2940	119	0
1	C	2925	0	2940	118	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	70	98	98	20	0
3	C	35	49	49	8	0
All	All	8883	147	8967	355	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 20.

The worst 5 of 355 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:THR:HG23	1:A:476:LEU:HD21	1.65	0.78
1:B:215:THR:HG23	1:B:476:LEU:HD21	1.65	0.78
1:C:215:THR:HG23	1:C:476:LEU:HD21	1.65	0.75
1:C:260:HIS:O	1:C:264:VAL:HG23	1.87	0.75
1:B:260:HIS:O	1:B:264:VAL:HG23	1.87	0.74

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	366/826 (44%)	358 (98%)	8 (2%)	0	100	100
1	B	366/826 (44%)	358 (98%)	8 (2%)	0	100	100
1	C	366/826 (44%)	358 (98%)	8 (2%)	0	100	100
All	All	1098/2478 (44%)	1074 (98%)	24 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	309/716 (43%)	307 (99%)	2 (1%)	86	91
1	B	309/716 (43%)	307 (99%)	2 (1%)	86	91
1	C	309/716 (43%)	307 (99%)	2 (1%)	86	91
All	All	927/2148 (43%)	921 (99%)	6 (1%)	92	91

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	321[B]	ARG
1	C	321[A]	ARG
1	C	321[B]	ARG
1	A	321[B]	ARG
1	A	321[A]	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	328	ASN
1	B	328	ASN
1	C	328	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 3 are monoatomic - leaving 3 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	Y01	C	901	-	38,38,38	1.73	9 (23%)	57,57,57	2.37	24 (42%)
3	Y01	A	902	-	38,38,38	1.73	9 (23%)	57,57,57	2.37	24 (42%)
3	Y01	A	903	-	38,38,38	1.74	9 (23%)	57,57,57	2.37	24 (42%)

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	Y01	C	901	-	-	12/19/77/77	0/4/4/4
3	Y01	A	902	-	-	12/19/77/77	0/4/4/4
3	Y01	A	903	-	-	12/19/77/77	0/4/4/4

The worst 5 of 27 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	901	Y01	CAT-CBH	-4.55	1.45	1.54
3	A	903	Y01	CAT-CBH	-4.54	1.45	1.54
3	A	902	Y01	CAT-CBH	-4.53	1.45	1.54
3	A	903	Y01	CAK-CBD	-4.32	1.45	1.53
3	A	902	Y01	CAK-CBD	-4.26	1.45	1.53

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

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	902	Y01	CAK-CAI-CAZ	-6.67	112.76	125.06
3	C	901	Y01	CAK-CAI-CAZ	-6.66	112.77	125.06
3	A	903	Y01	CAK-CAI-CAZ	-6.66	112.78	125.06
3	A	903	Y01	CAT-CBH-CBF	6.57	117.91	108.73
3	A	902	Y01	CAT-CBH-CBF	6.54	117.86	108.73

There are no chirality outliers.

5 of 36 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	902	Y01	OAG-CAY-OAW-CBC
3	A	903	Y01	OAG-CAY-OAW-CBC
3	C	901	Y01	OAG-CAY-OAW-CBC
3	A	902	Y01	CAM-CAY-OAW-CBC
3	A	903	Y01	CAM-CAY-OAW-CBC

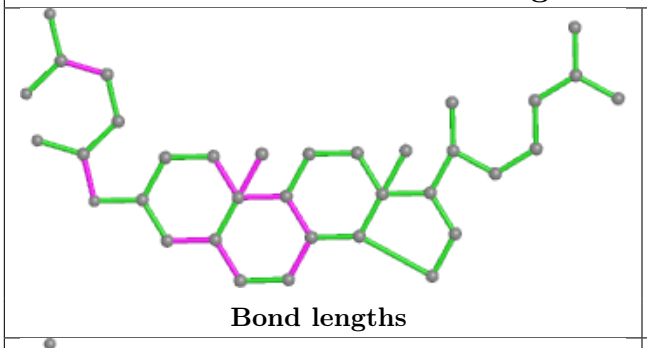
There are no ring outliers.

3 monomers are involved in 27 short contacts:

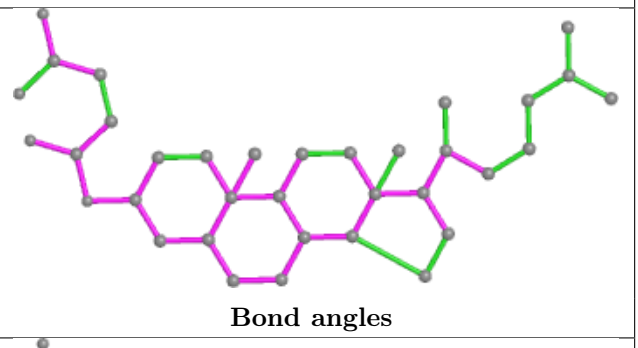
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	901	Y01	8	0
3	A	902	Y01	11	0
3	A	903	Y01	10	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

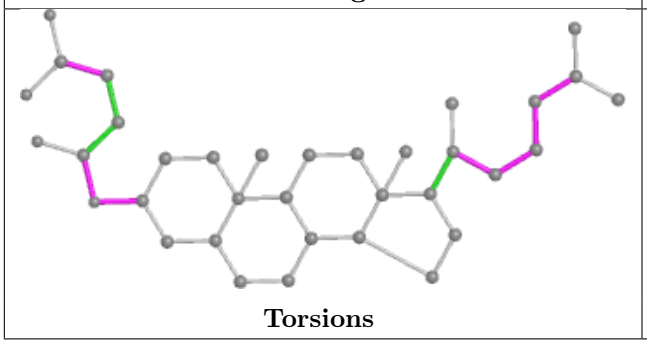
Ligand Y01 C 901



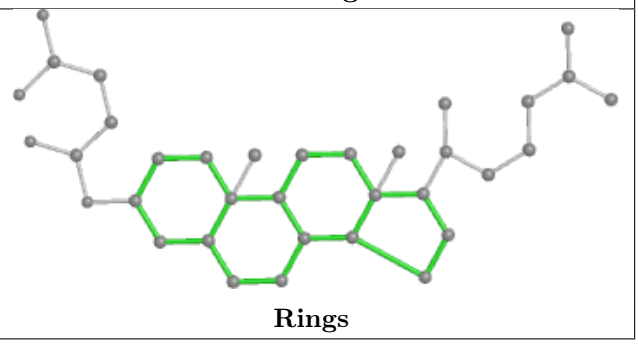
Bond lengths



Bond angles

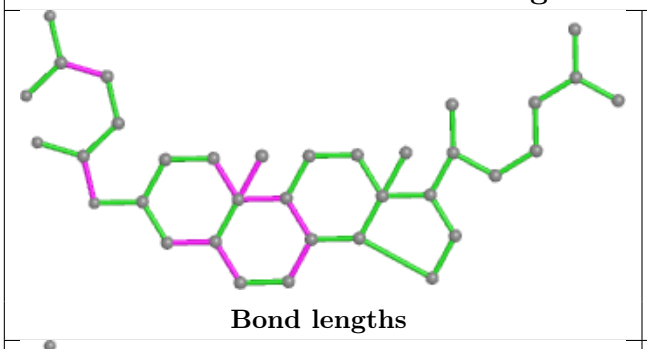


Torsions

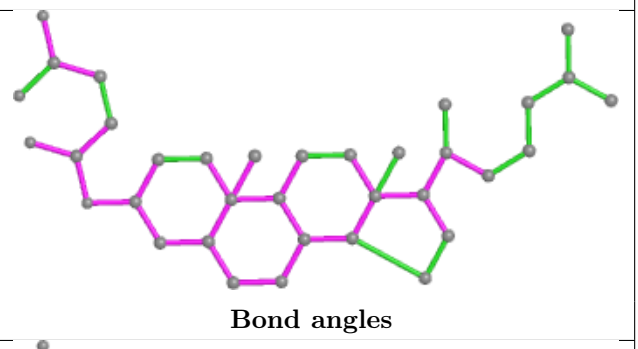


Rings

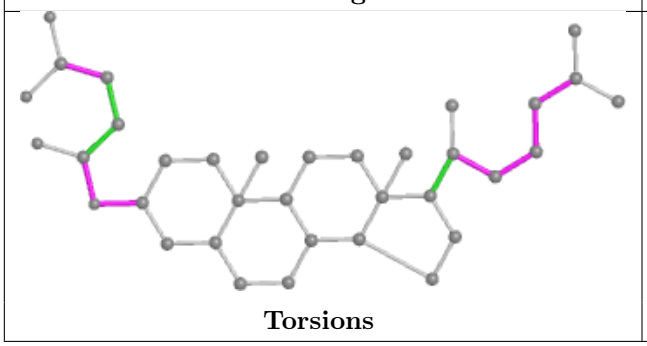
Ligand Y01 A 902



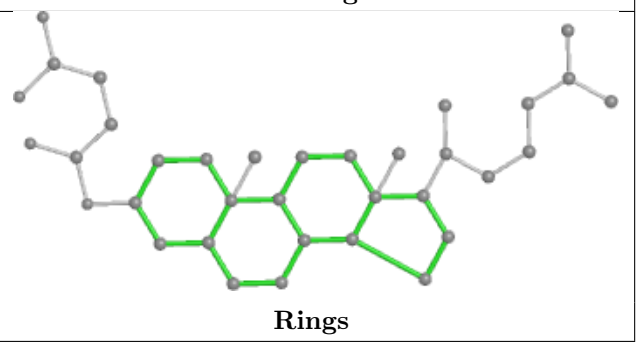
Bond lengths



Bond angles

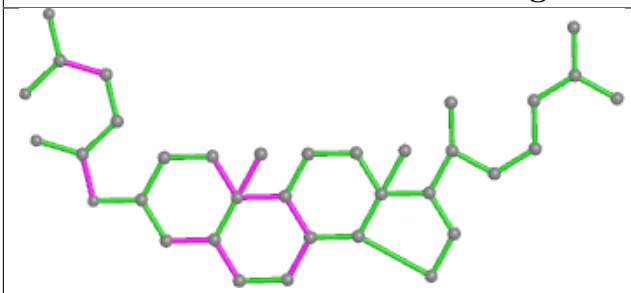


Torsions

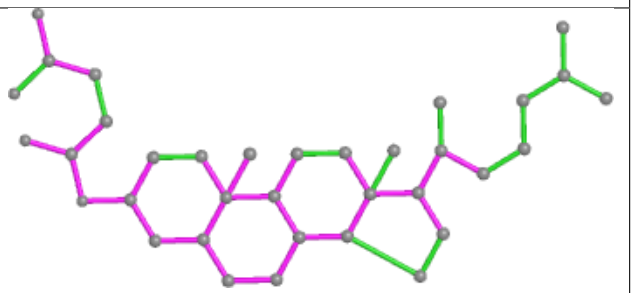


Rings

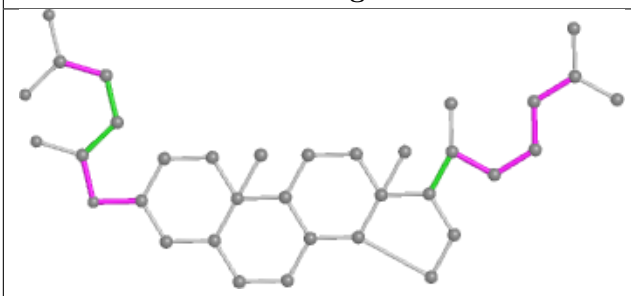
Ligand Y01 A 903



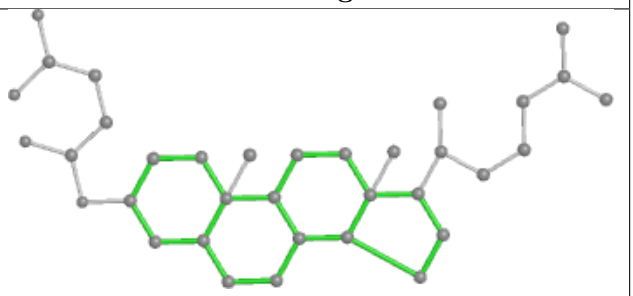
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Map visualisation

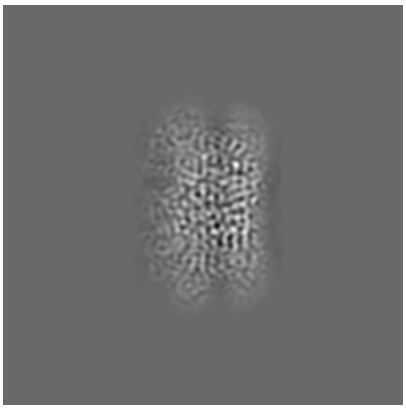
This section contains visualisations of the EMDB entry EMD-34303. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

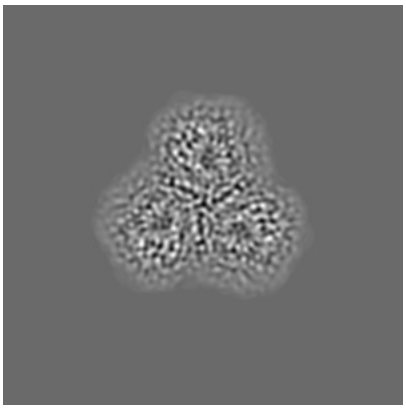
6.1 Orthogonal projections

6.1.1 Primary map

X

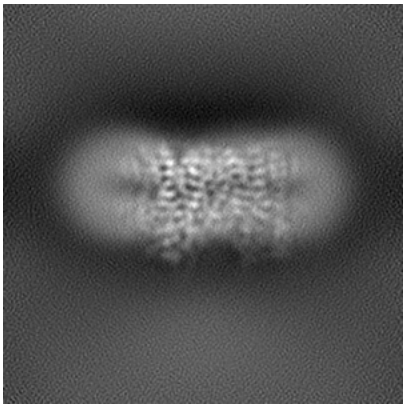


Y

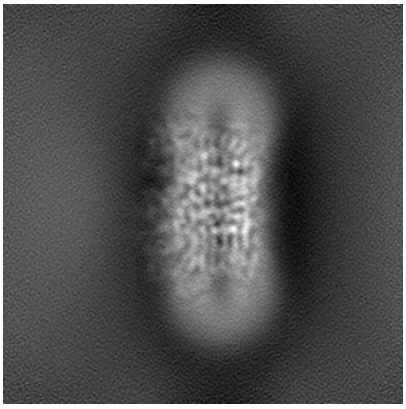


Z

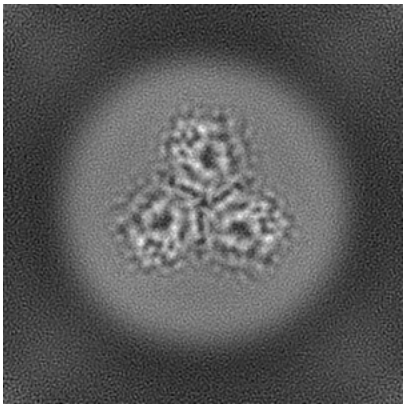
6.1.2 Raw map



X



Y



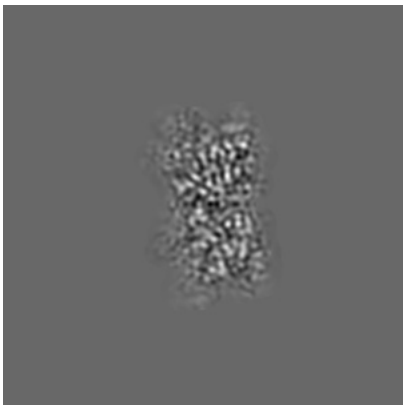
Z

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

6.2 Central slices (i)

6.2.1 Primary map

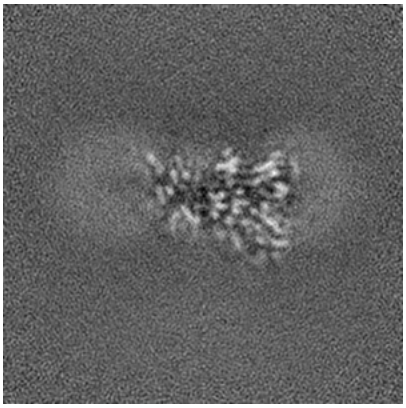
X Index: 120



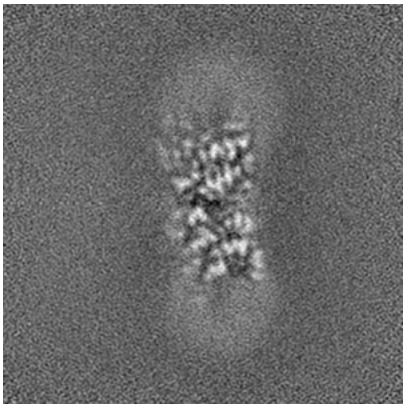
Y Index: 120

Z Index: 120

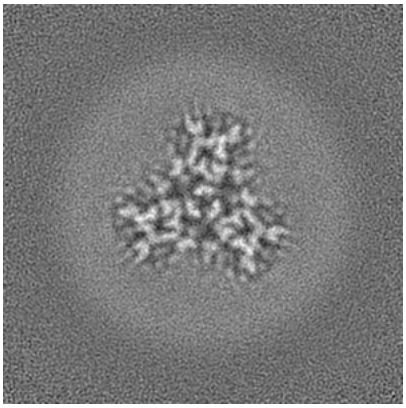
6.2.2 Raw map



X Index: 120



Y Index: 120



Z Index: 120

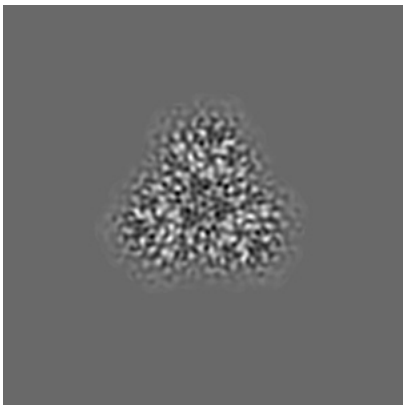
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map

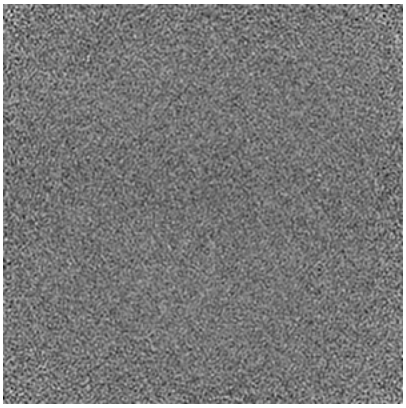
X Index: 112

Y Index: 100

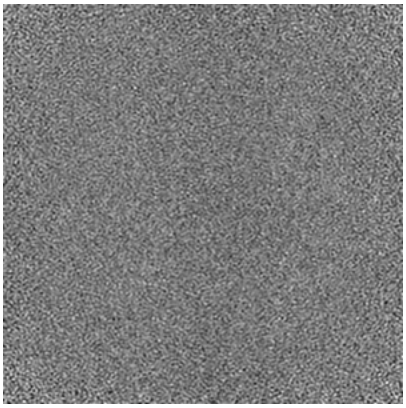


Z Index: 139

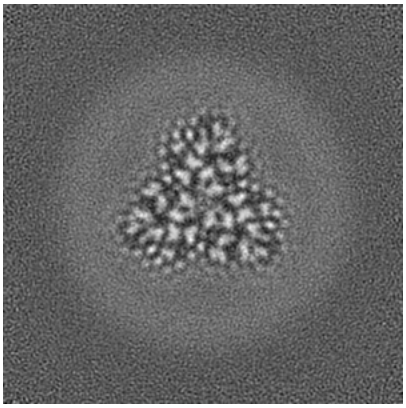
6.3.2 Raw map



X Index: 0



Y Index: 0

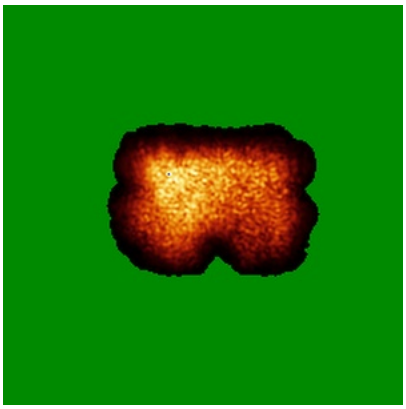


Z Index: 140

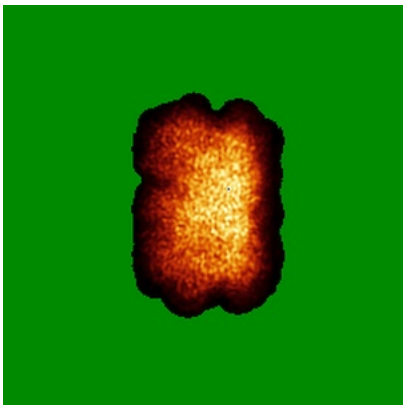
The images above show the largest variance slices of the map in three orthogonal directions.

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

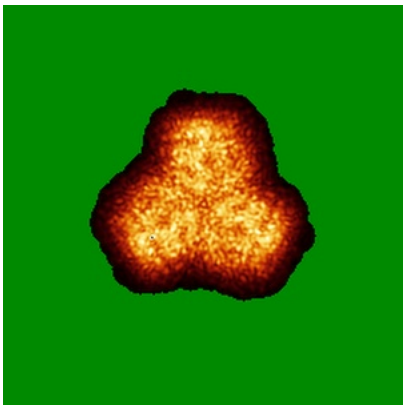
6.4.1 Primary map



X

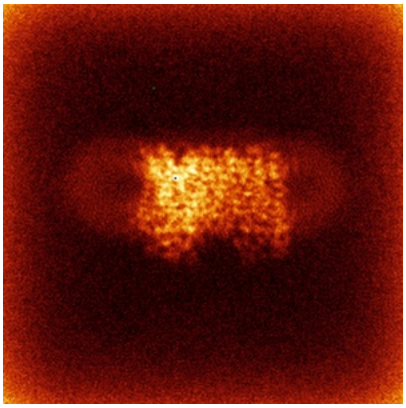


Y

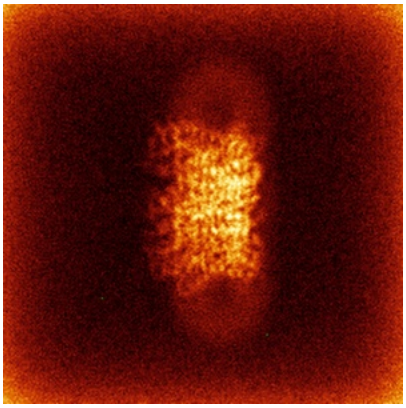


Z

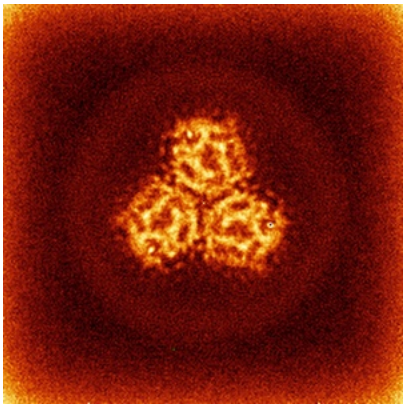
6.4.2 Raw map



X



Y

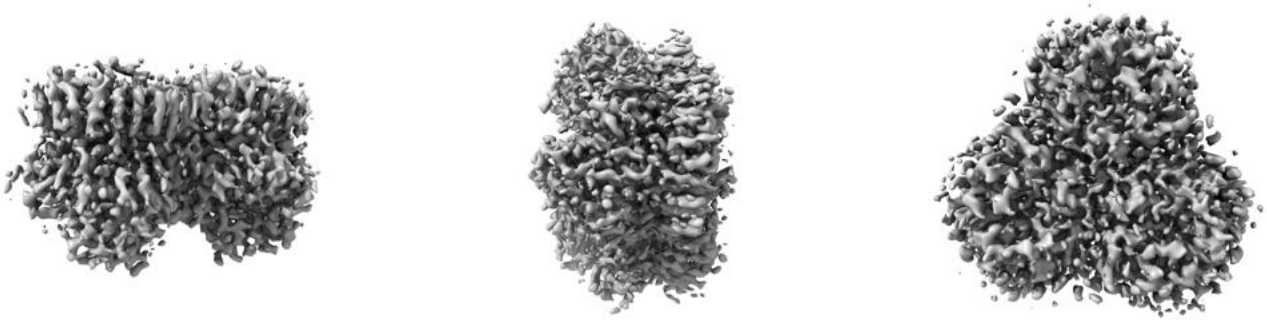


Z

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)

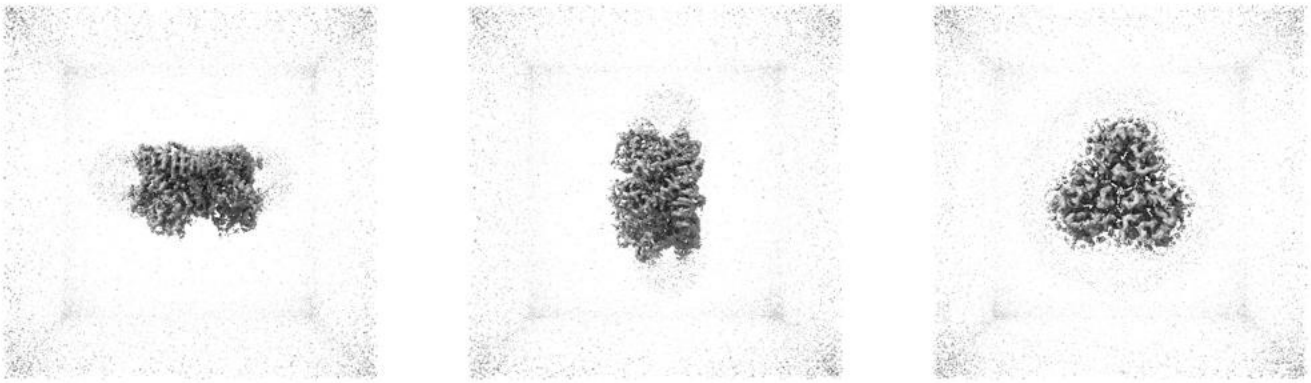
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.176. 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



X Y Z

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.

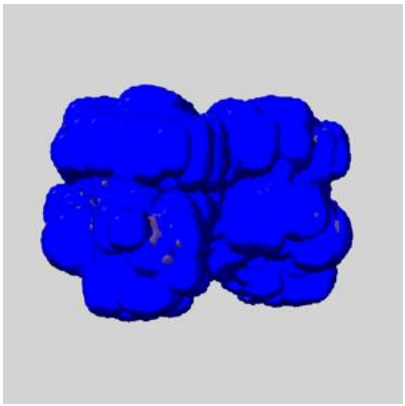
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

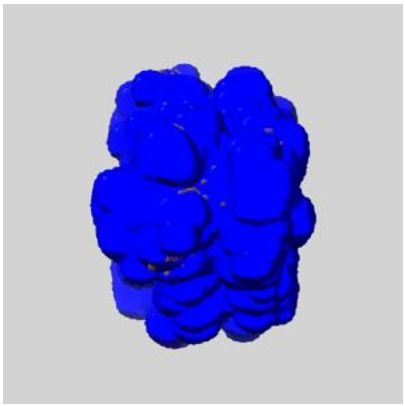
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

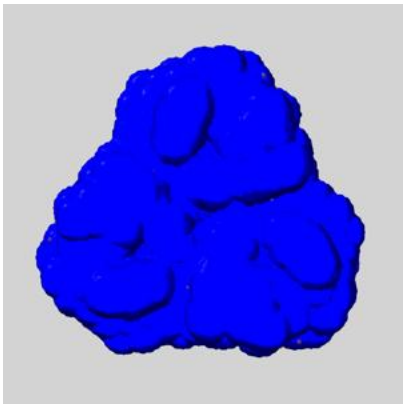
6.6.1 emd_34303_msk_1.map (i)



X



Y

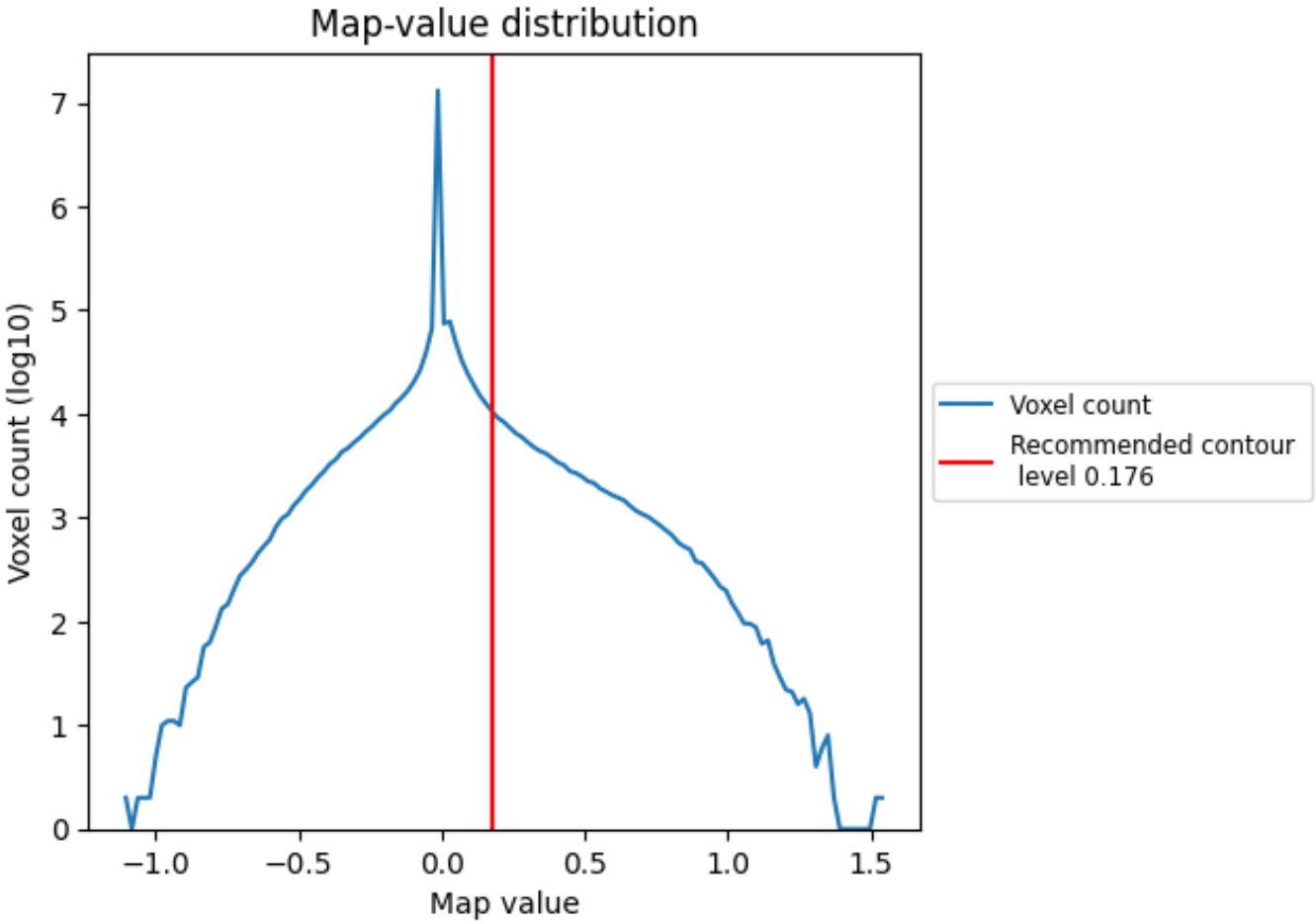


Z

7 Map analysis

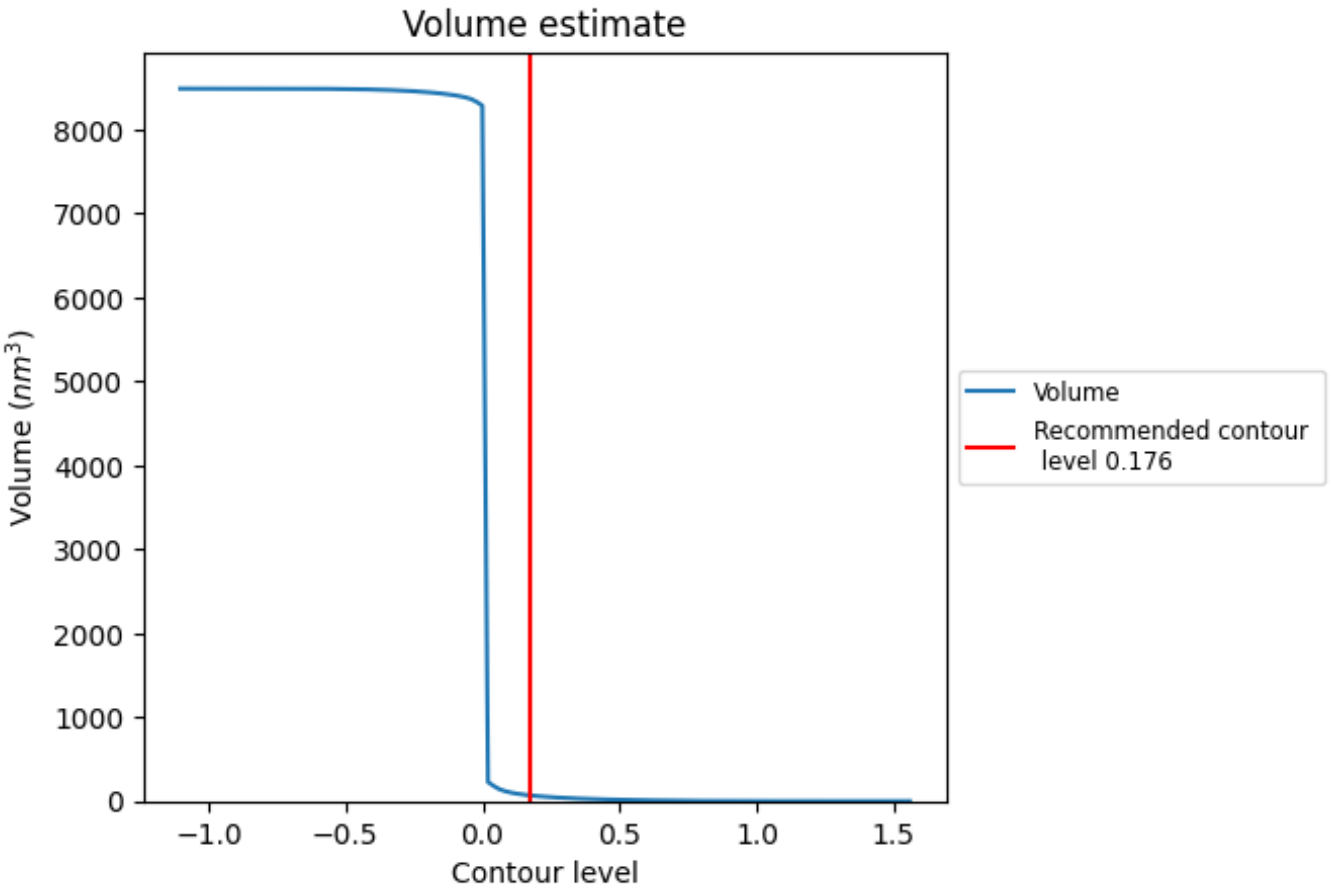
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

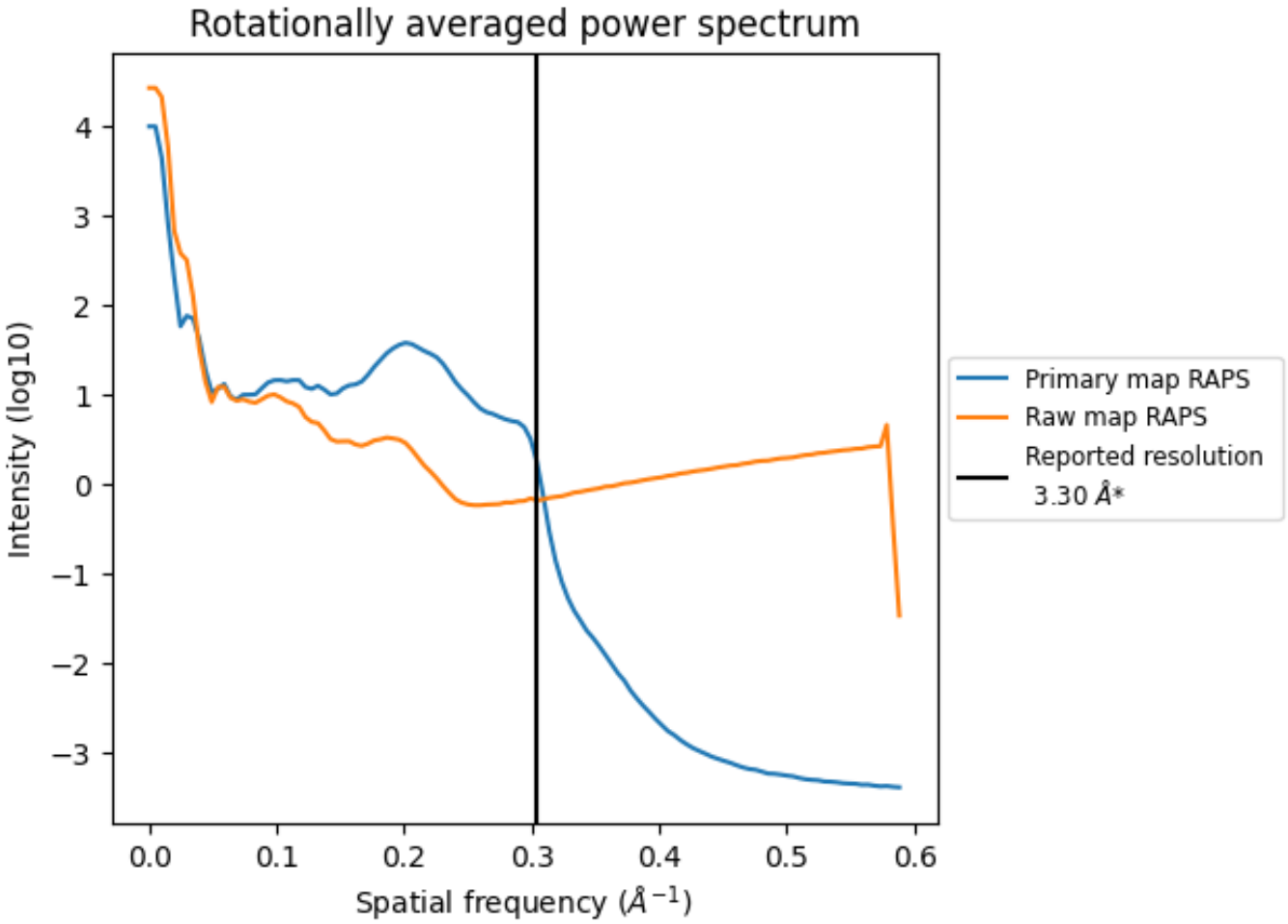
7.2 Volume estimate (i)



The volume at the recommended contour level is 68 nm^3; this corresponds to an approximate mass of 61 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

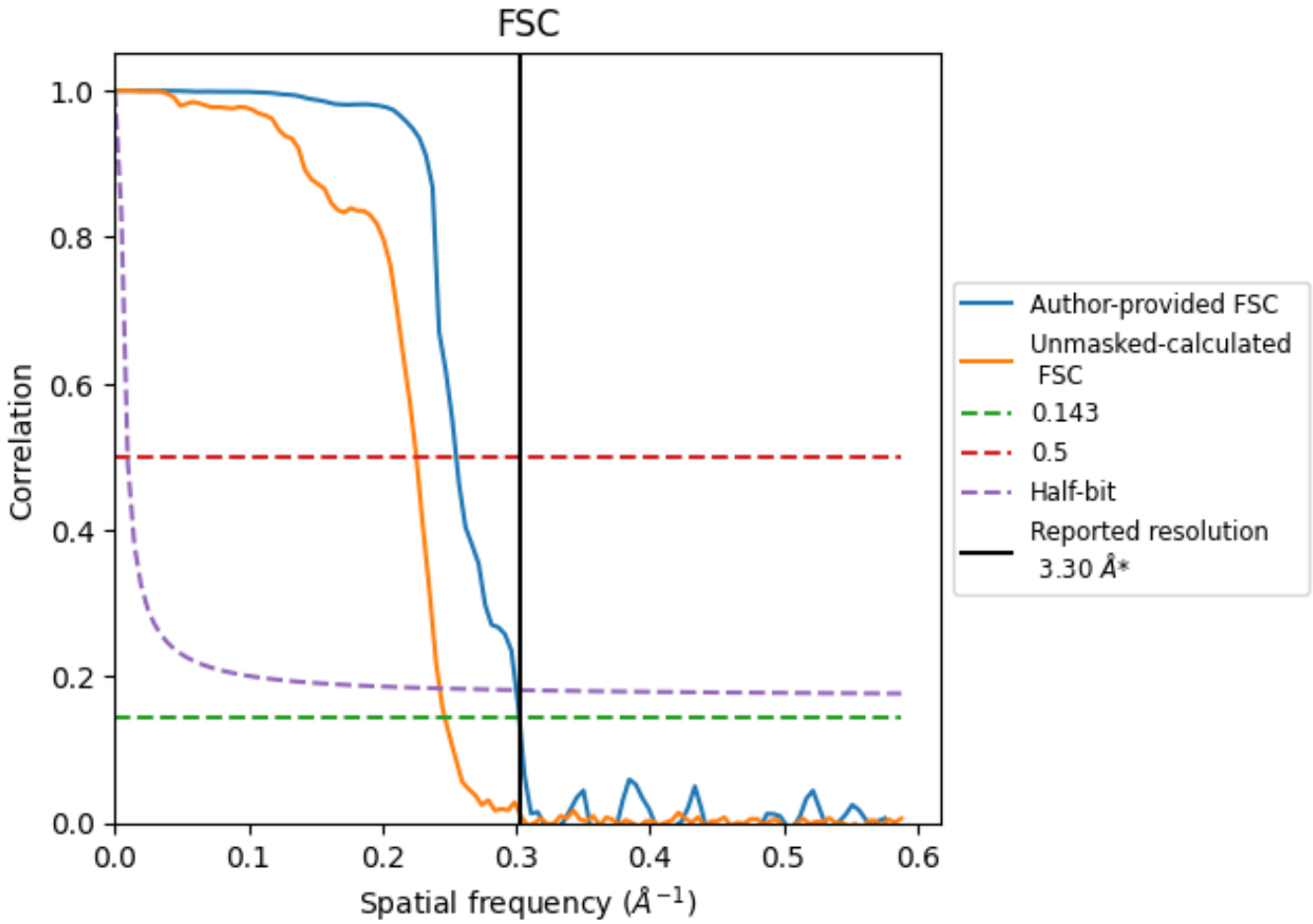


*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.303 Å^{-1}

8.2 Resolution estimates (i)

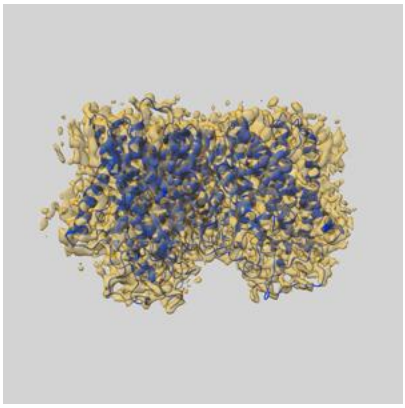
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.31	3.92	3.33
Unmasked-calculated*	4.05	4.43	4.12

*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 4.05 differs from the reported value 3.3 by more than 10 %

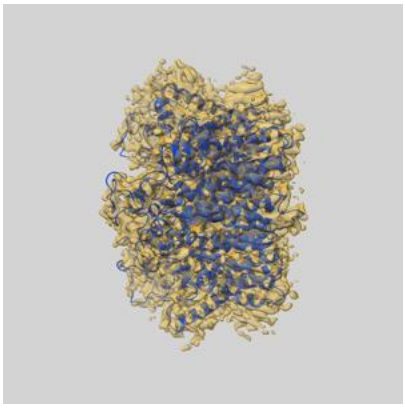
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-34303 and PDB model 8GW6. Per-residue inclusion information can be found in section 3 on page 8.

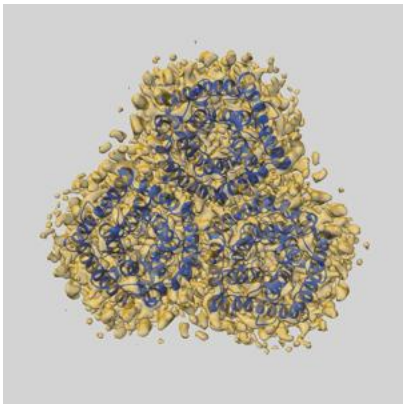
9.1 Map-model overlay



X



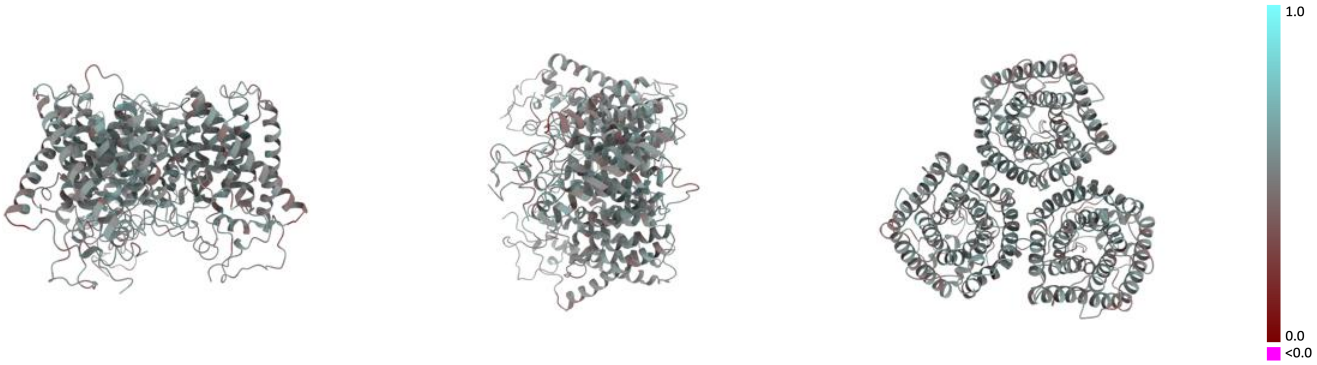
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.176 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

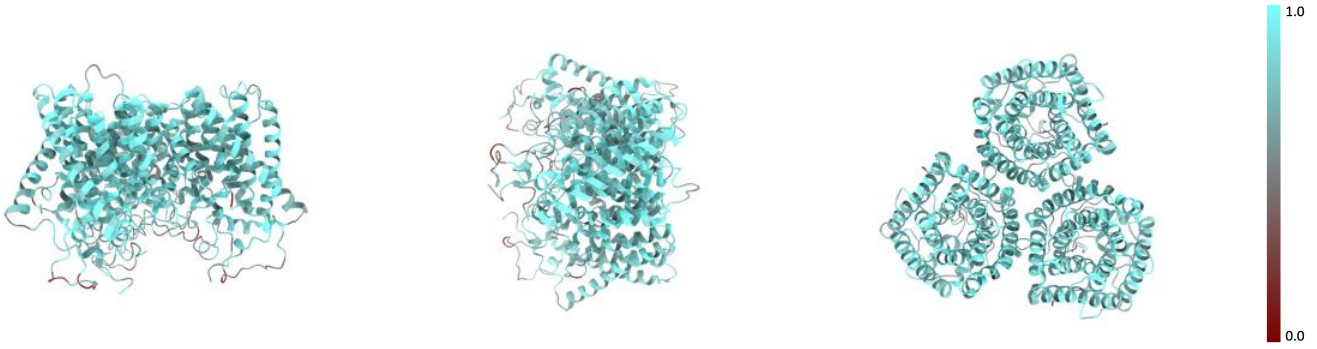
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

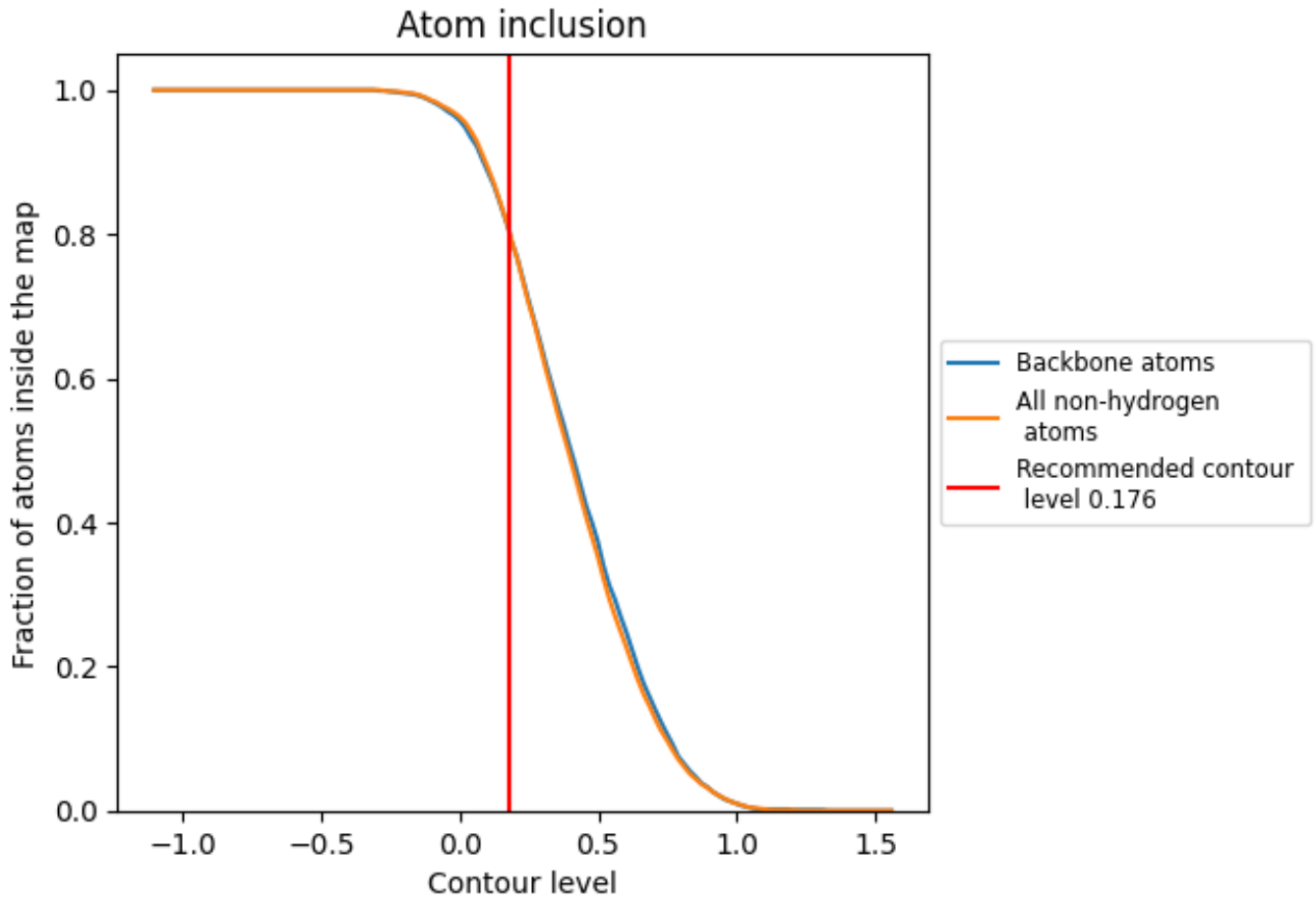
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.176).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 81% 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 (0.176) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8090	0.4980
A	0.8090	0.4980
B	0.8070	0.4970
C	0.8070	0.4970