wwPDB EM Validation Summary Report

Jun 16, 2024 – 12:15 AM JST

PDB ID	:	8WUI
EMDB ID	:	EMD-37855
Title	:	SKOR D312N L271P double mutation
Authors	:	Gao, X.; Sun, T.; Lu, Y.; Jia, Y.; Xu, X.; Zhang, Y.; Fu, P.; Yang, G.
Deposited on	:	2023-10-20
Resolution	:	3.40 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:

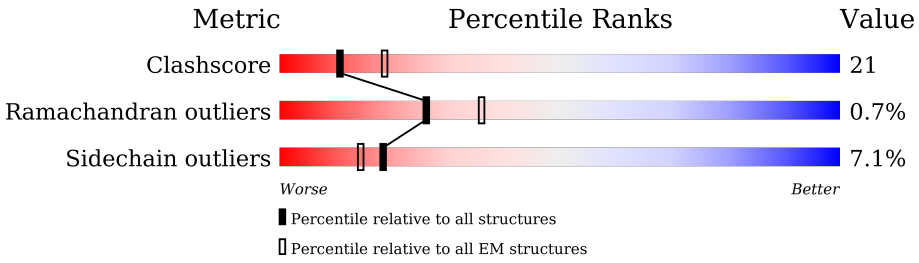
EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

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 3.40 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	838	26% 34% 18% • 45%
1	B	838	27% 34% 19% • 46%
1	C	838	27% 34% 19% • 45%
1	D	838	27% 34% 19% • 46%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 15340 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 Potassium channel SKOR.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	449	Total	C	N	O	S	0	0
			3706	2432	612	639	23		
1	A	464	Total	C	N	O	S	0	0
			3832	2510	637	662	23		
1	D	449	Total	C	N	O	S	0	0
			3706	2432	612	639	23		
1	C	464	Total	C	N	O	S	0	0
			3832	2510	637	662	23		

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-9	MET	-	initiating methionine	UNP Q9M8S6
B	-8	ASP	-	expression tag	UNP Q9M8S6
B	-7	TYR	-	expression tag	UNP Q9M8S6
B	-6	LYS	-	expression tag	UNP Q9M8S6
B	-5	ASP	-	expression tag	UNP Q9M8S6
B	-4	ASP	-	expression tag	UNP Q9M8S6
B	-3	ASP	-	expression tag	UNP Q9M8S6
B	-2	ASP	-	expression tag	UNP Q9M8S6
B	-1	LYS	-	expression tag	UNP Q9M8S6
B	0	HIS	-	expression tag	UNP Q9M8S6
B	271	PRO	LEU	engineered mutation	UNP Q9M8S6
B	312	ASN	ASP	engineered mutation	UNP Q9M8S6
A	-9	MET	-	initiating methionine	UNP Q9M8S6
A	-8	ASP	-	expression tag	UNP Q9M8S6
A	-7	TYR	-	expression tag	UNP Q9M8S6
A	-6	LYS	-	expression tag	UNP Q9M8S6
A	-5	ASP	-	expression tag	UNP Q9M8S6
A	-4	ASP	-	expression tag	UNP Q9M8S6
A	-3	ASP	-	expression tag	UNP Q9M8S6
A	-2	ASP	-	expression tag	UNP Q9M8S6
A	-1	LYS	-	expression tag	UNP Q9M8S6
A	0	HIS	-	expression tag	UNP Q9M8S6

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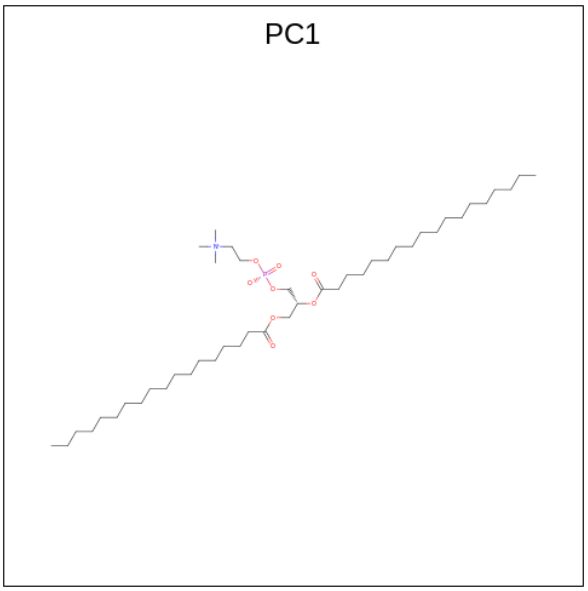
Chain	Residue	Modelled	Actual	Comment	Reference
A	271	PRO	LEU	engineered mutation	UNP Q9M8S6
A	312	ASN	ASP	engineered mutation	UNP Q9M8S6
D	-9	MET	-	initiating methionine	UNP Q9M8S6
D	-8	ASP	-	expression tag	UNP Q9M8S6
D	-7	TYR	-	expression tag	UNP Q9M8S6
D	-6	LYS	-	expression tag	UNP Q9M8S6
D	-5	ASP	-	expression tag	UNP Q9M8S6
D	-4	ASP	-	expression tag	UNP Q9M8S6
D	-3	ASP	-	expression tag	UNP Q9M8S6
D	-2	ASP	-	expression tag	UNP Q9M8S6
D	-1	LYS	-	expression tag	UNP Q9M8S6
D	0	HIS	-	expression tag	UNP Q9M8S6
D	271	PRO	LEU	engineered mutation	UNP Q9M8S6
D	312	ASN	ASP	engineered mutation	UNP Q9M8S6
C	-9	MET	-	initiating methionine	UNP Q9M8S6
C	-8	ASP	-	expression tag	UNP Q9M8S6
C	-7	TYR	-	expression tag	UNP Q9M8S6
C	-6	LYS	-	expression tag	UNP Q9M8S6
C	-5	ASP	-	expression tag	UNP Q9M8S6
C	-4	ASP	-	expression tag	UNP Q9M8S6
C	-3	ASP	-	expression tag	UNP Q9M8S6
C	-2	ASP	-	expression tag	UNP Q9M8S6
C	-1	LYS	-	expression tag	UNP Q9M8S6
C	0	HIS	-	expression tag	UNP Q9M8S6
C	271	PRO	LEU	engineered mutation	UNP Q9M8S6
C	312	ASN	ASP	engineered mutation	UNP Q9M8S6

- Molecule 2 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (three-letter code: PC1) (formula: $C_{44}H_{88}NO_8P$).



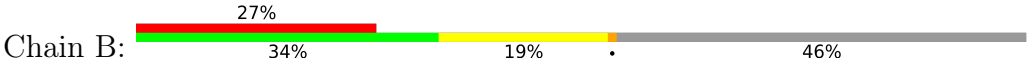
Mol	Chain	Residues	Atoms	AltConf
2	B	1	Total C 17 17	0
2	B	1	Total C 17 17	0
2	B	1	Total C 17 17	0
2	A	1	Total C 17 17	0
2	A	1	Total C 17 17	0
2	A	1	Total C O P 30 21 8 1	0
2	A	1	Total C 17 17	0
2	D	1	Total C 17 17	0
2	D	1	Total C 17 17	0
2	D	1	Total C 17 17	0
2	C	1	Total C O P 30 21 8 1	0
2	C	1	Total C 17 17	0
2	C	1	Total C 17 17	0
2	C	1	Total C 17 17	0

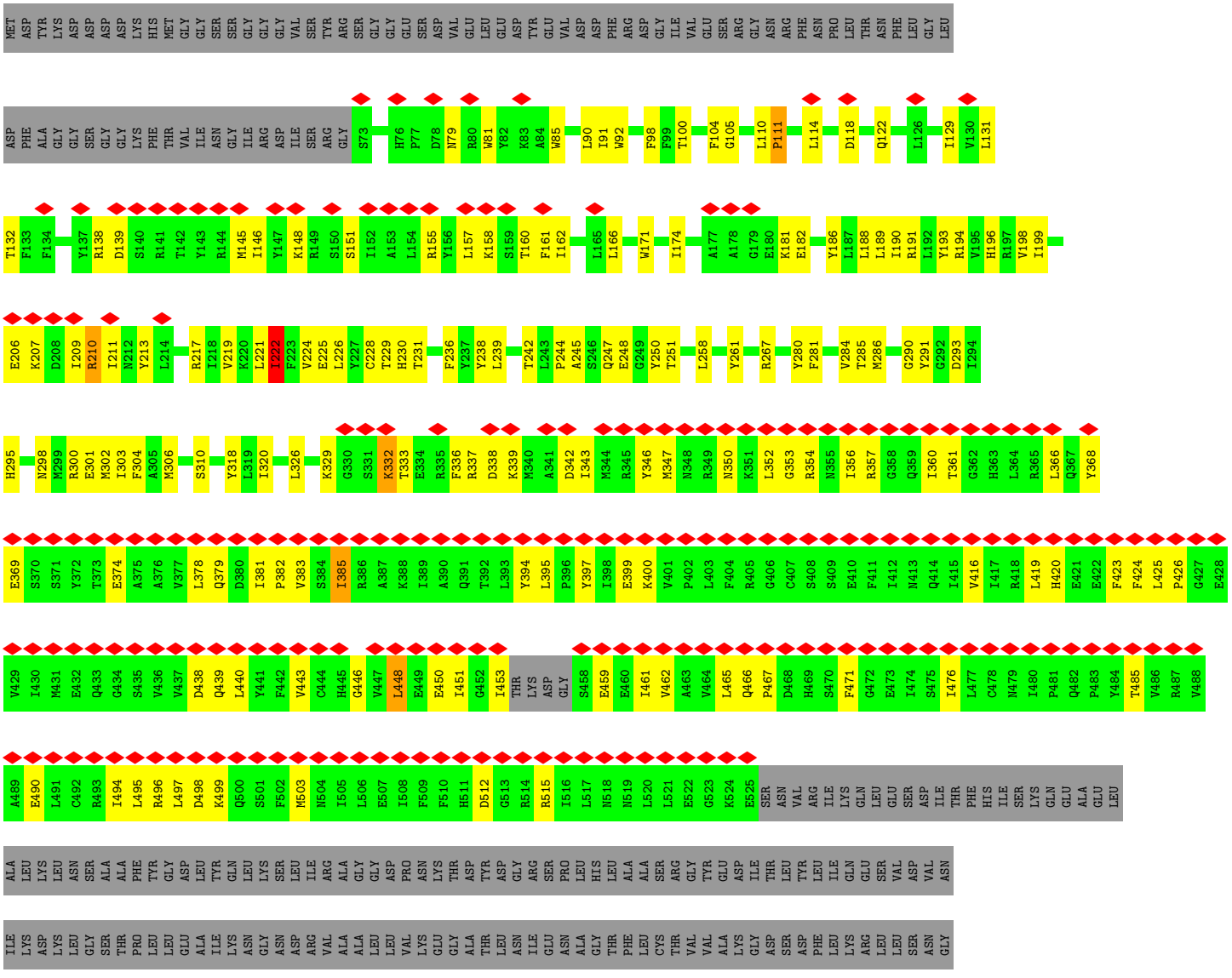
3 Residue-property plots (i)

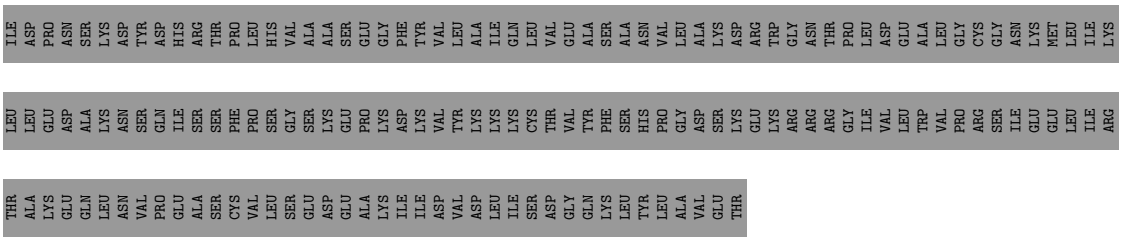
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

Chain B:

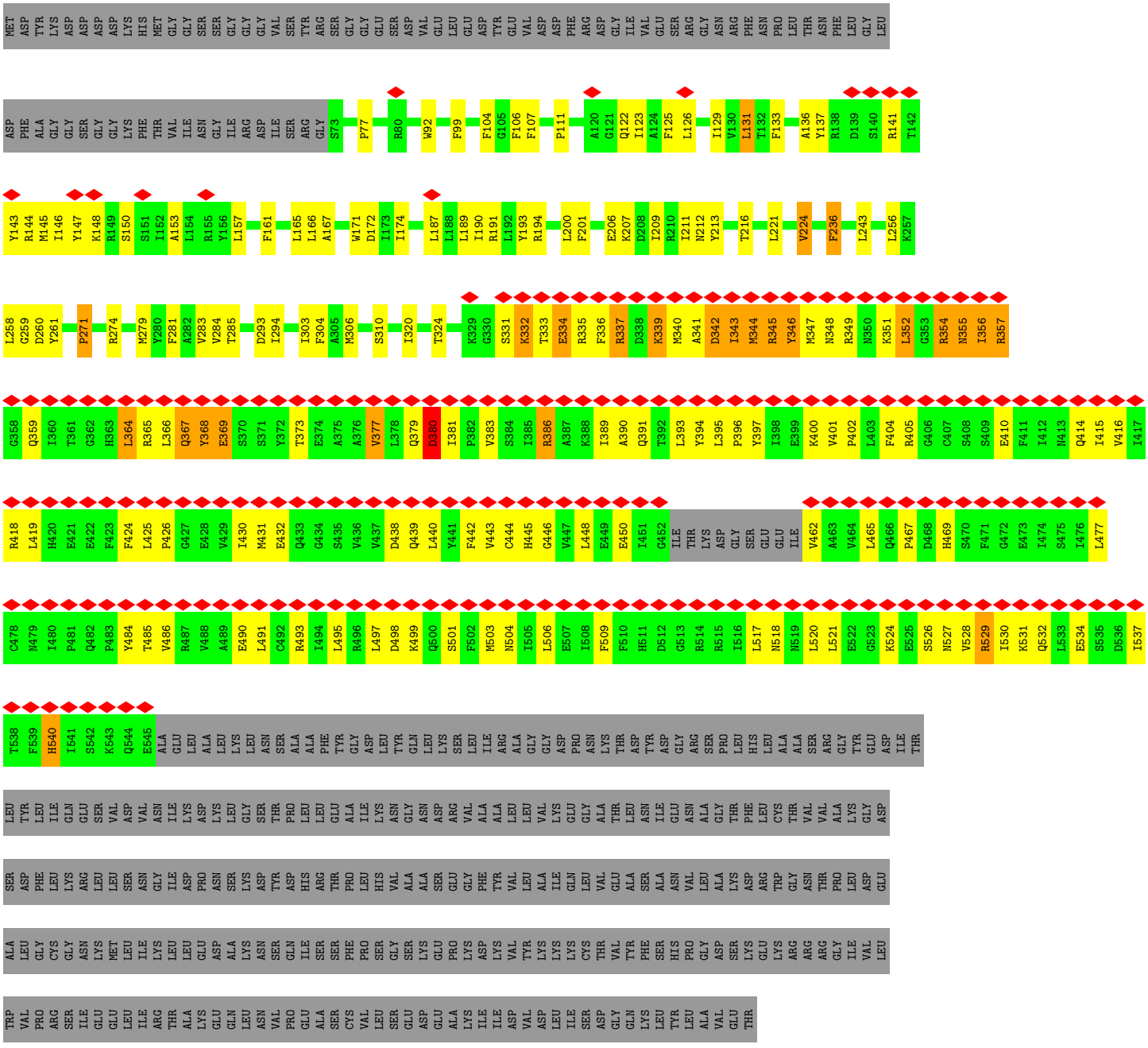






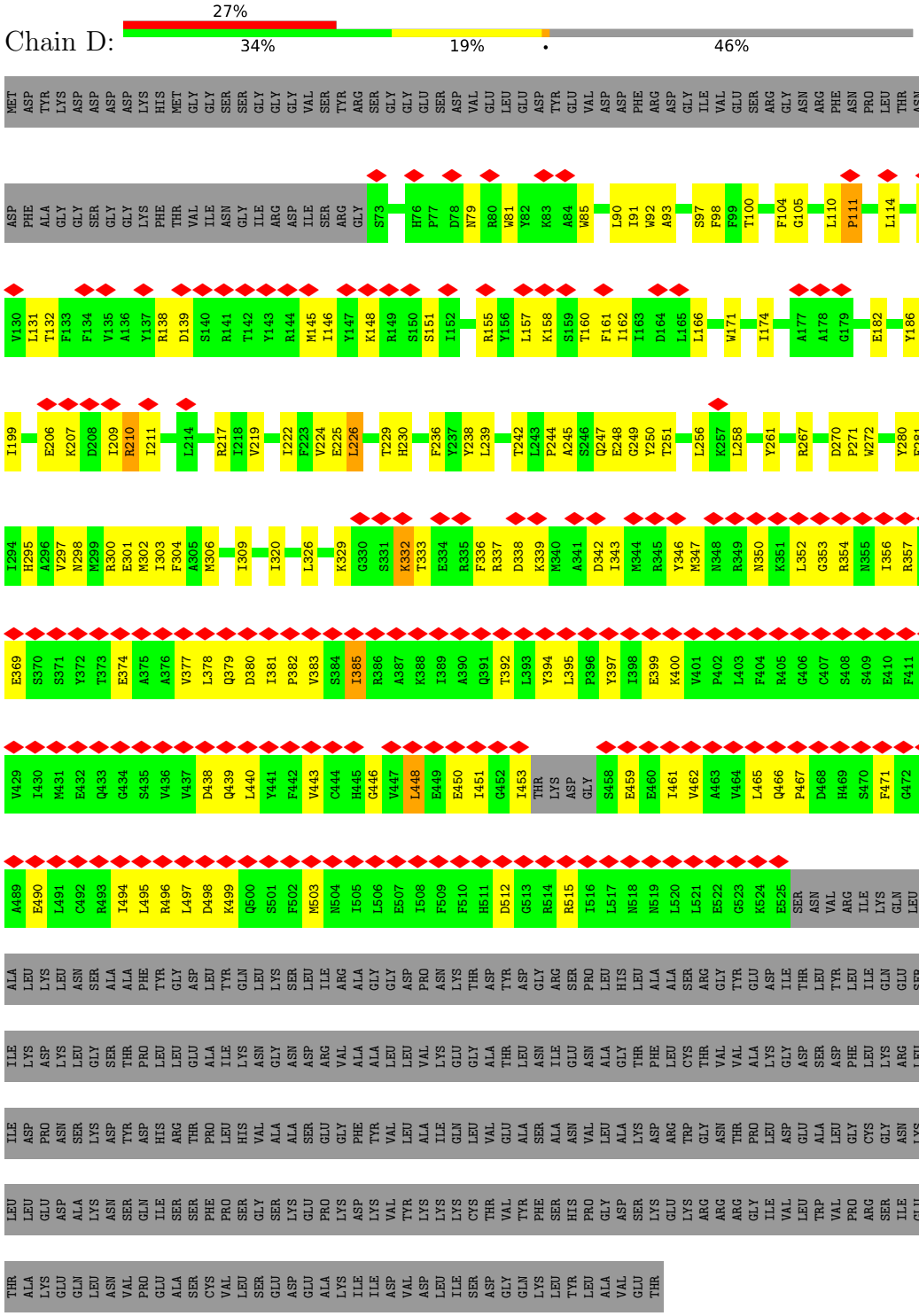
• Molecule 1: Potassium channel SKOR

Chain A:



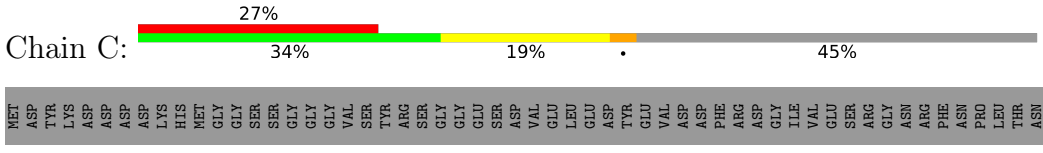
• Molecule 1: Potassium channel SKOR

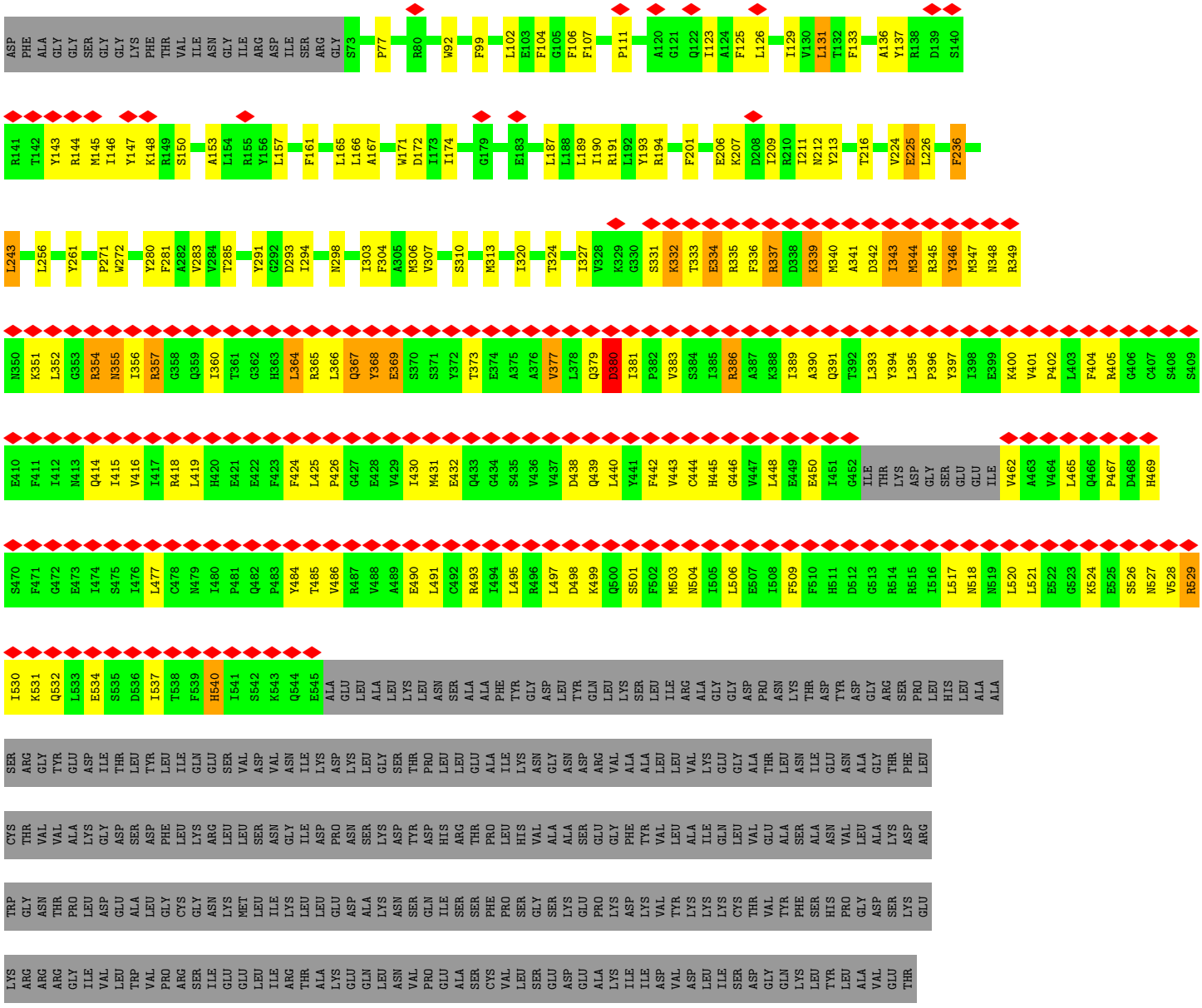
Chain D:



- Molecule 1: Potassium channel SKOR

Chain C:




ASP PHE ALA GLY GLY SER GLY GLY LYS PHE THR VAL ILE ASN GLY ILE ARG ASP ILE SER ARG GLY S73 P77 R80 W92 F99 L102 E103 F104 G105 F106 F107 P111 A120 G121 Q122 I123 A124 F125 L126 I129 V130 L131 T132 F133 A136 Y137 R138 D139 S140
R141 T142 Y143 R144 M145 I146 Y147 K148 R149 S150 A153 L154 R155 Y156 L157 F161 L165 L166 A167 W171 D172 I173 I174 G179 E183 L187 L188 L189 I190 R191 L192 Y193 R194 F201 E206 K207 D208 I209 R210 I211 N212 Y213 T216 V224 E225 L226 F236
L243 L256 Y261 P271 W272 Y280 F281 A282 V283 V284 T285 Y291 G292 D293 I294 N298 I303 F304 A305 M306 V307 S310 M313 I320 T324 I327 V328 K329 G330 S331 K332 T333 E334 R335 F336 R337 D338 K339 M340 A341 D342 I343 M344 R345 Y346 M347 N348 R349
N350 K351 L352 G353 R354 N355 I356 R357 G358 Q359 I360 T361 G362 H363 L364 R365 L366 Q367 Y368 E369 S370 S371 Y372 T373 E374 A375 A376 V377 L378 Q379 D380 I381 P382 V383 S384 I385 R386 A387 K388 I389 A390 Q391 T392 L393 Y394 L395 P396 Y397 I398 E399 K400 V401 P402 L403 F404 R405 G406 C407 S408 S409
E410 F411 I412 N413 Q414 I415 V416 I417 R418 L419 H420 E421 E422 F423 F424 L425 P426 G427 E428 V429 I430 M431 E432 Q433 G434 S435 V436 V437 D438 Q439 L440 Y441 F442 V443 C444 H445 G446 V447 L448 E449 E450 I451 G452 ILE THR LYS ASP GLY SER GLU GLU ILE V462 A463 V464 L465 Q466 P467 D468 H469
S470 F471 G472 E473 I474 S475 I476 L477 C478 N479 I480 P481 Q482 P483 Y484 T485 V486 R487 V488 A489 E490 L491 C492 R493 I494 L495 R496 L497 D498 K499 Q500 S501 F502 M503 N504 I505 L506 E507 I508 F509 F510 H511 D512 G513 R514 R515 I516 L517 N518 N519 L520 L521 E522 G523 K524 E525 S526 N527 V528 R529
I530 K531 Q532 L533 E534 S535 D536 I537 T538 F539 H540 I541 S542 K543 Q544 E545 ALA GLU LEU ALA LEU LYS LEU ASN SER ALA ALA PHE TYR GLY ASP LEU TYR GLN LEU LYS SER LEU ILE ARG ALA GLY GLY ASP PRO ASN LYS THR ASP TYR ASP GLY ARG SER PRO LEU HIS LEU ALA ALA
SER ARG GLY TYR GLU ASP ILE THR LEU TYR LEU ILE GLN GLU SER VAL ASP VAL ASN ILE LYS ASP LYS LEU GLY SER THR PRO LEU LEU GLU ALA ILE LYS ASN GLY ASN ASP ARG VAL ALA ALA LEU LEU LEU VAL LYS GLU GLY ALA THR LEU ASN ILE GLU ASN ALA GLY THR PHE LEU
CYS THR VAL VAL ALA LYS GLY ASP SER ASP PHE LEU LYS ARG LEU LEU SER ASN GLY ILE ILE ASP PRO ASN SER LYS ASP TYR ASP HIS ARG THR PRO LEU HIS VAL ALA ALA SER GLU GLY PHE TYR VAL LEU ALA ILE GLN LEU VAL GLU ALA SER ALA ASN VAL LEU ALA LYS ASP ARG
TRP GLY ASN THR PRO LEU ASP GLU ALA LEU GLY CYS GLY ASN LYS MET LEU ILE LYS LEU LEU GLU ASP ALA LYS ASN SER GLN ILE SER SER PHE PRO SER GLY SER LYS GLU PRO LYS ASP LYS VAL TYR LYS LYS LYS CYS THR VAL TYR PHE SER HIS PRO GLY ASP SER LYS GLU
LYS ARG ARG GLY ILE VAL LEU TRP VAL PRO ARG SER ILE GLU GLU LEU ILE ARG THR ALA LYS GLU GLN LEU ASN VAL PRO GLU ALA SER CYS VAL LEU SER GLU ASP GLU ALA LYS ILE ILE ASP VAL ASP LEU ILE SER ASP GLY GLN LYS LEU TYR LEU ALA VAL GLU THR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	97040	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.795	Depositor
Minimum map value	-1.079	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.032	Depositor
Recommended contour level	0.184	Depositor
Map size (Å)	291.19998, 291.19998, 291.19998	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PC1

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	0.37	0/3925	0.56	3/5307 (0.1%)
1	B	0.30	0/3797	0.51	0/5136
1	C	0.37	0/3925	0.56	3/5307 (0.1%)
1	D	0.30	0/3797	0.52	0/5136
All	All	0.34	0/15444	0.54	6/20886 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	131	LEU	CA-CB-CG	8.22	134.21	115.30
1	A	131	LEU	CA-CB-CG	8.22	134.20	115.30
1	A	271	PRO	CA-N-CD	-6.05	103.03	111.50
1	C	271	PRO	CA-N-CD	-6.03	103.06	111.50
1	C	271	PRO	N-CD-CG	-5.31	95.23	103.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	380	ASP	Mainchain
1	C	380	ASP	Mainchain

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	3832	0	3881	218	0
1	B	3706	0	3754	181	0
1	C	3832	0	3881	201	0
1	D	3706	0	3754	190	0
2	A	81	0	123	32	0
2	B	51	0	90	24	0
2	C	81	0	123	34	0
2	D	51	0	90	20	0
All	All	15340	0	15696	644	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 21.

The worst 5 of 644 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:B:304:PHE:CD1	2:B:901:PC1:H2E1	1.15	1.66
1:C:272:TRP:HD1	2:C:902:PC1:C21	1.00	1.65
1:C:107:PHE:CE1	2:C:901:PC1:H11	1.16	1.62
1:A:346:TYR:CE2	1:D:378:LEU:HD22	1.33	1.57
1:C:107:PHE:CZ	2:C:901:PC1:H11	1.38	1.55

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	460/838 (55%)	422 (92%)	35 (8%)	3 (1%)	22 55
1	B	445/838 (53%)	418 (94%)	23 (5%)	4 (1%)	17 49
1	C	460/838 (55%)	425 (92%)	32 (7%)	3 (1%)	22 55
1	D	445/838 (53%)	419 (94%)	23 (5%)	3 (1%)	22 55
All	All	1810/3352 (54%)	1684 (93%)	113 (6%)	13 (1%)	26 55

5 of 13 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	161	PHE
1	D	161	PHE
1	B	210	ARG
1	A	355	ASN
1	D	210	ARG

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	415/727 (57%)	372 (90%)	43 (10%)	7 25
1	B	400/727 (55%)	386 (96%)	14 (4%)	36 65
1	C	415/727 (57%)	371 (89%)	44 (11%)	6 24
1	D	400/727 (55%)	386 (96%)	14 (4%)	36 65
All	All	1630/2908 (56%)	1515 (93%)	115 (7%)	18 44

5 of 115 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	193	TYR
1	C	386	ARG

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Mol	Chain	Res	Type
1	C	137	TYR
1	C	380	ASP
1	C	355	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	363	HIS
1	C	359	GLN
1	D	379	GLN
1	D	295	HIS
1	D	439	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

14 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	$\#\|Z\| > 2$
2	PC1	D	903	-	16,16,53	0.11	0	15,15,61	0.08	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PC1	A	903	-	29,29,53	0.45	0	33,34,61	0.57	1 (3%)
2	PC1	C	901	-	29,29,53	0.46	0	33,34,61	0.70	1 (3%)
2	PC1	C	903	-	16,16,53	0.13	0	15,15,61	0.12	0
2	PC1	A	904	-	16,16,53	0.12	0	15,15,61	0.09	0
2	PC1	B	902	-	16,16,53	0.11	0	15,15,61	0.09	0
2	PC1	D	902	-	16,16,53	0.11	0	15,15,61	0.08	0
2	PC1	C	902	-	16,16,53	0.12	0	15,15,61	0.09	0
2	PC1	B	903	-	16,16,53	0.13	0	15,15,61	0.08	0
2	PC1	B	901	-	16,16,53	0.11	0	15,15,61	0.09	0
2	PC1	C	904	-	16,16,53	0.11	0	15,15,61	0.07	0
2	PC1	D	901	-	16,16,53	0.13	0	15,15,61	0.09	0
2	PC1	A	901	-	16,16,53	0.09	0	15,15,61	0.06	0
2	PC1	A	902	-	16,16,53	0.11	0	15,15,61	0.07	0

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
2	PC1	D	903	-	-	8/14/14/57	-
2	PC1	A	903	-	-	14/31/31/57	-
2	PC1	C	901	-	-	14/31/31/57	-
2	PC1	C	903	-	-	11/14/14/57	-
2	PC1	A	904	-	-	6/14/14/57	-
2	PC1	B	902	-	-	11/14/14/57	-
2	PC1	D	902	-	-	8/14/14/57	-
2	PC1	C	902	-	-	7/14/14/57	-
2	PC1	B	903	-	-	9/14/14/57	-
2	PC1	B	901	-	-	8/14/14/57	-
2	PC1	C	904	-	-	10/14/14/57	-
2	PC1	D	901	-	-	8/14/14/57	-
2	PC1	A	901	-	-	6/14/14/57	-
2	PC1	A	902	-	-	10/14/14/57	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	903	PC1	O12-P-O14	2.46	120.31	110.68
2	C	901	PC1	O12-P-O14	2.25	119.48	110.68

There are no chirality outliers.

5 of 130 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	903	PC1	C1-O11-P-O12
2	A	903	PC1	C1-O11-P-O14
2	A	903	PC1	C1-O11-P-O13
2	C	901	PC1	C1-O11-P-O14
2	C	901	PC1	C22-C21-O21-C2

There are no ring outliers.

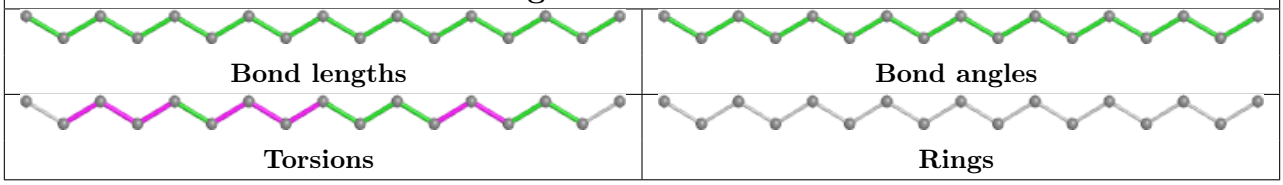
14 monomers are involved in 110 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	903	PC1	6	0
2	A	903	PC1	16	0
2	C	901	PC1	17	0
2	C	903	PC1	10	0
2	A	904	PC1	1	0
2	B	902	PC1	12	0
2	D	902	PC1	9	0
2	C	902	PC1	4	0
2	B	903	PC1	2	0
2	B	901	PC1	13	0
2	C	904	PC1	3	0
2	D	901	PC1	5	0
2	A	901	PC1	3	0
2	A	902	PC1	12	0

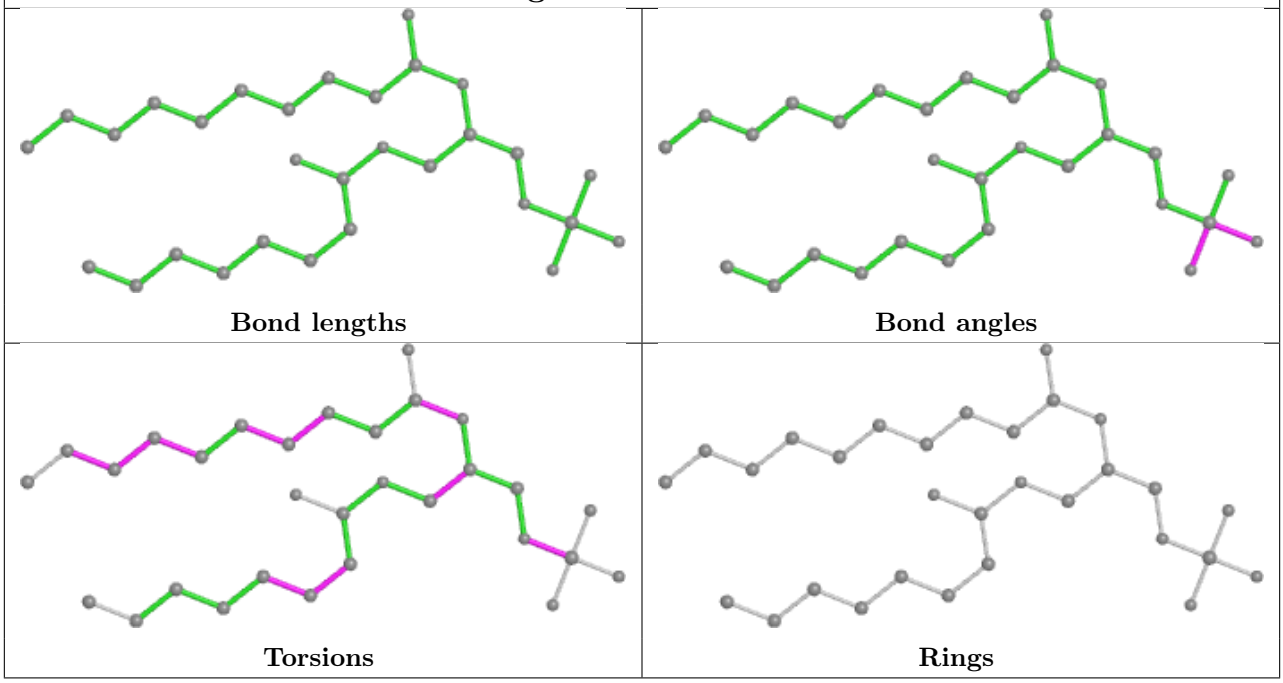
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

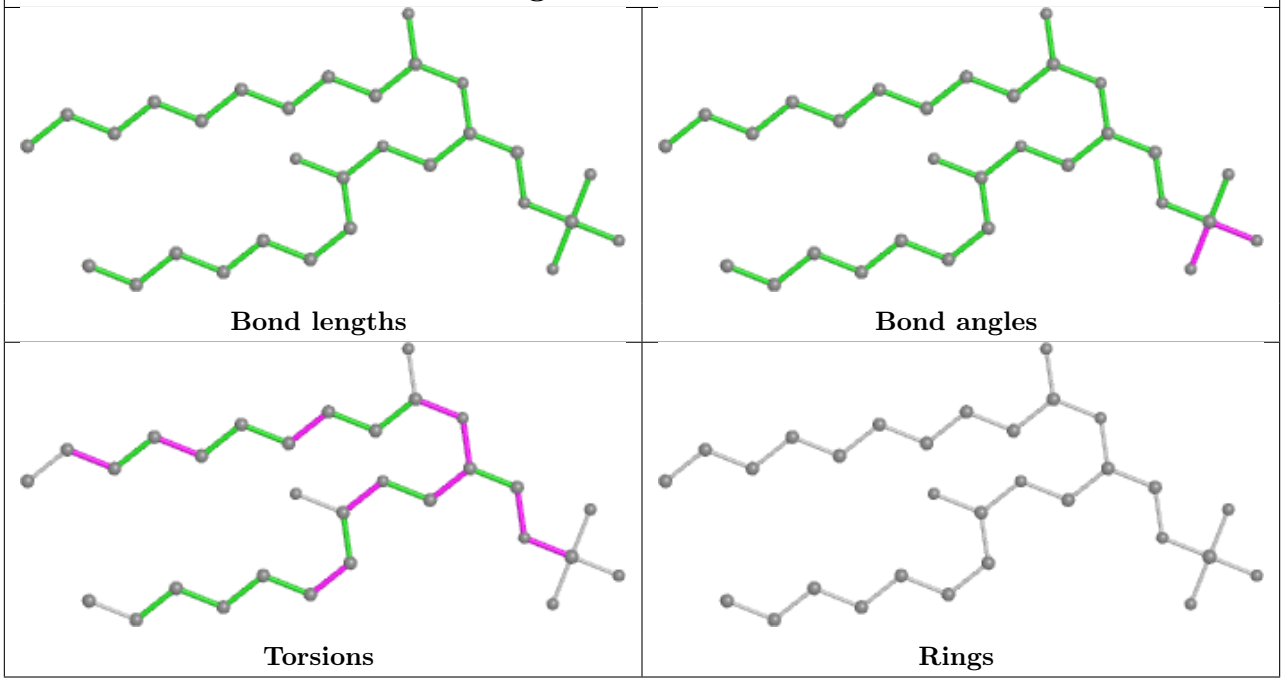
Ligand PC1 D 903

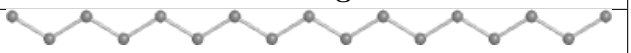


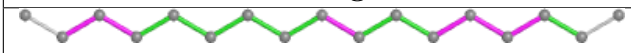
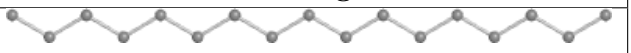
Ligand PC1 A 903

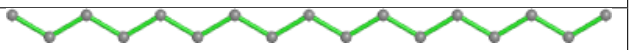
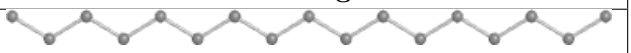


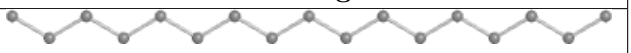
Ligand PC1 C 901

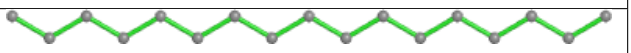
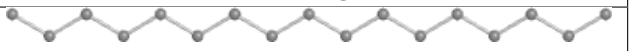


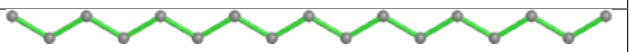
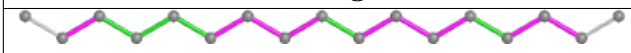
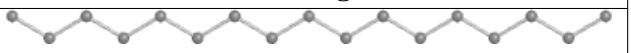
Ligand PC1 C 903	
 Bond lengths	 Bond angles
 Torsions	 Rings

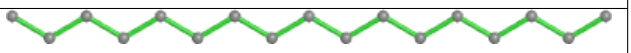
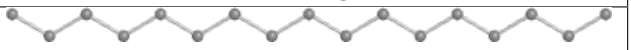
Ligand PC1 A 904	
 Bond lengths	 Bond angles
 Torsions	 Rings

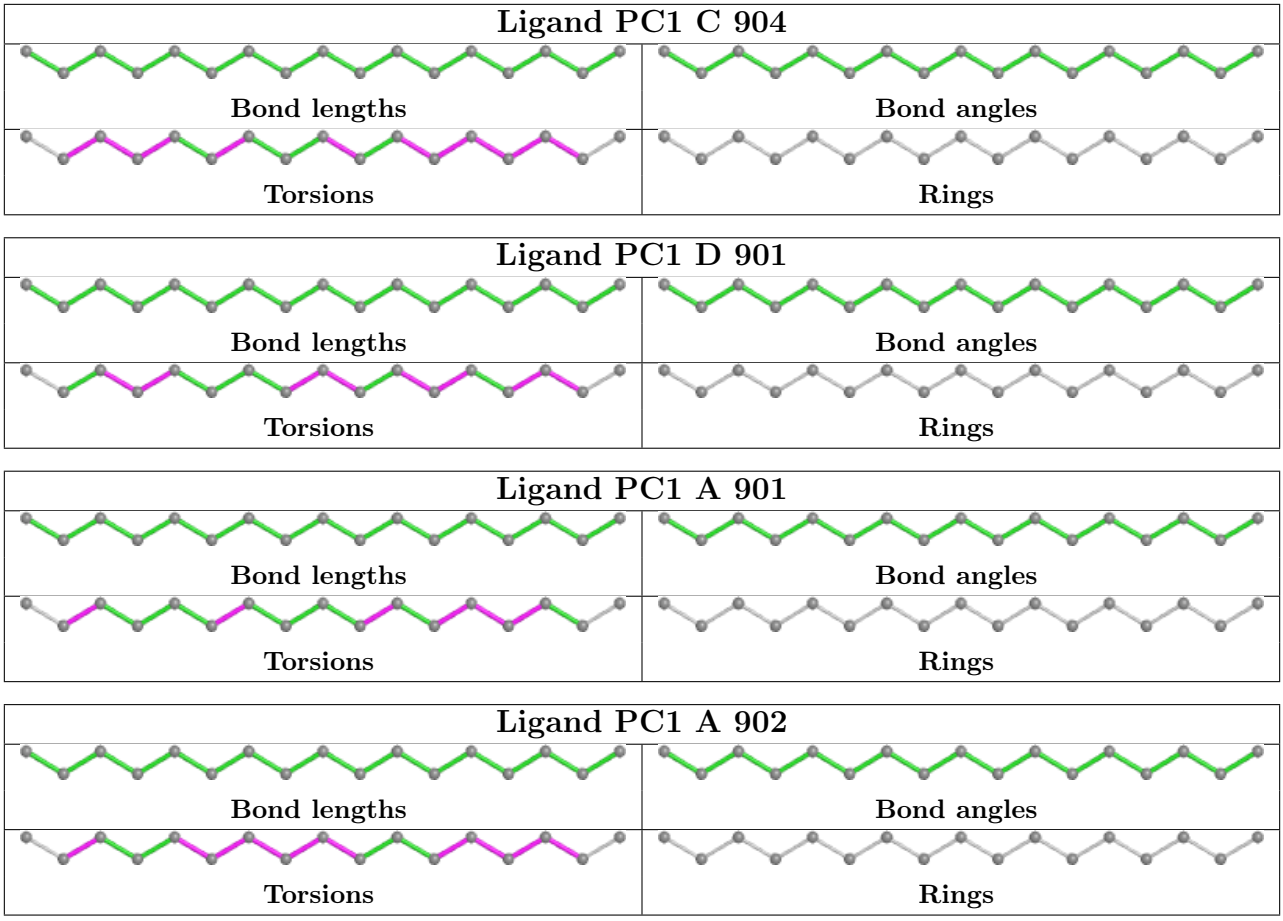
Ligand PC1 B 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 D 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 C 902	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 B 903	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand PC1 B 901	
 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.

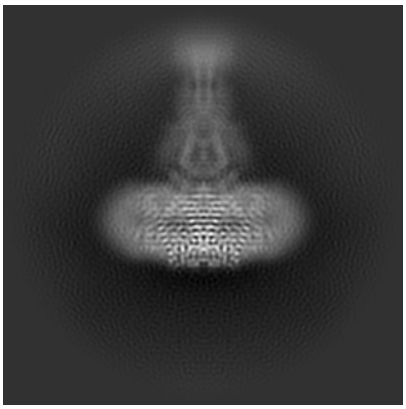
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-37855. These allow visual inspection of the internal detail of the map and identification of artifacts.

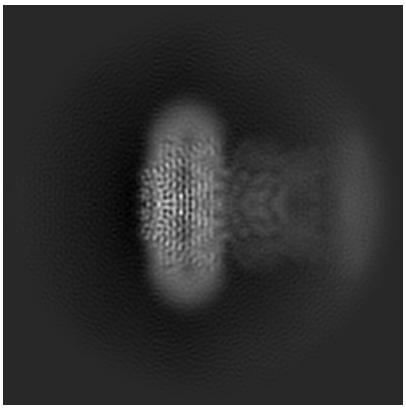
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

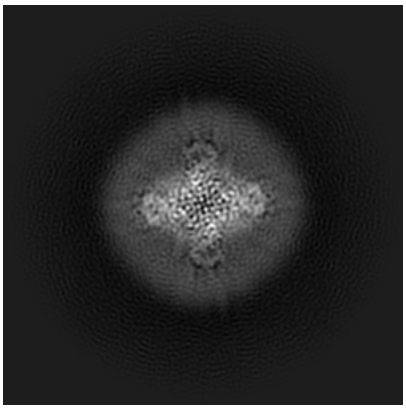
6.1.1 Primary map



X

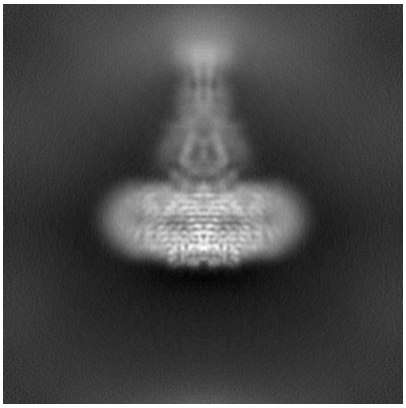


Y

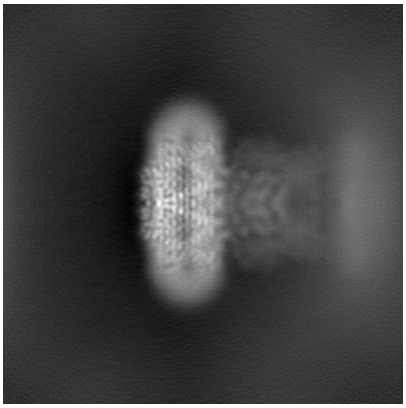


Z

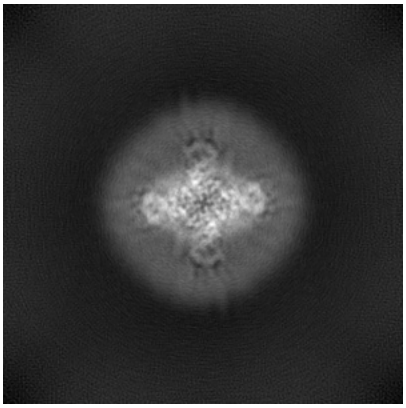
6.1.2 Raw map



X



Y

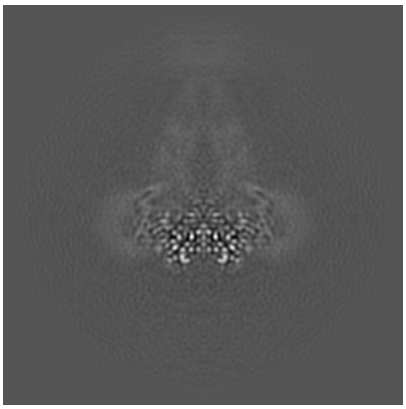


Z

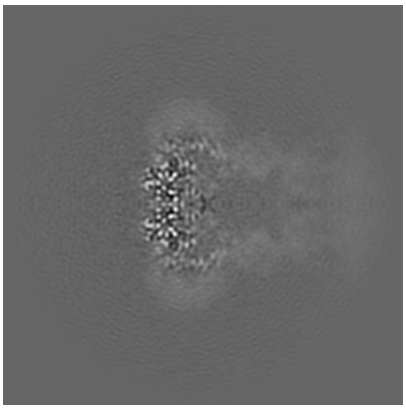
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

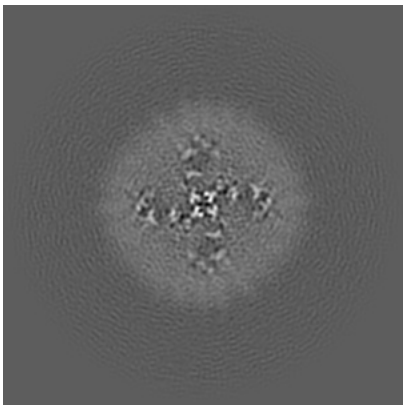
6.2.1 Primary map



X Index: 140

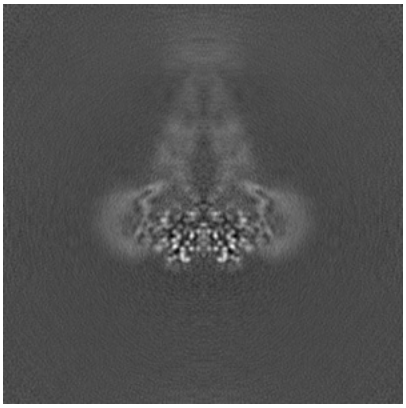


Y Index: 140

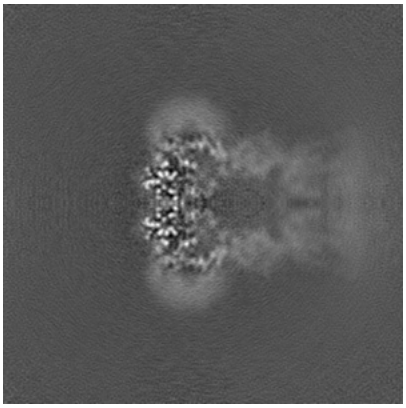


Z Index: 140

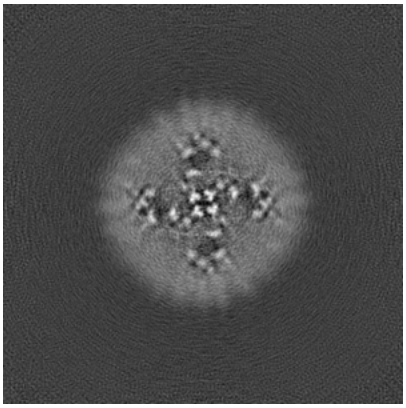
6.2.2 Raw map



X Index: 140



Y Index: 140

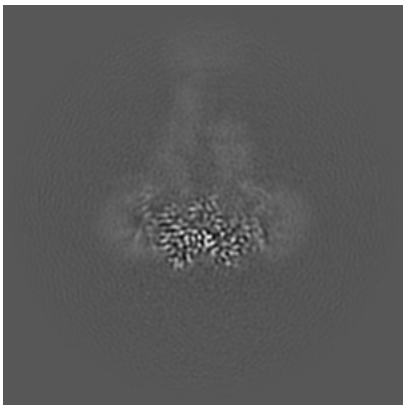


Z Index: 140

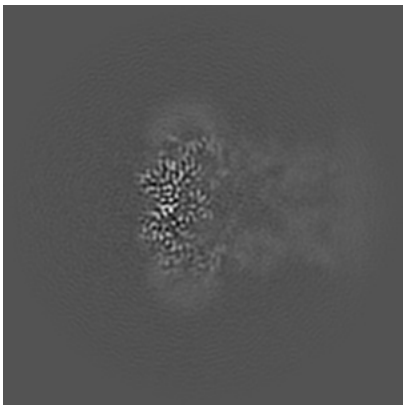
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

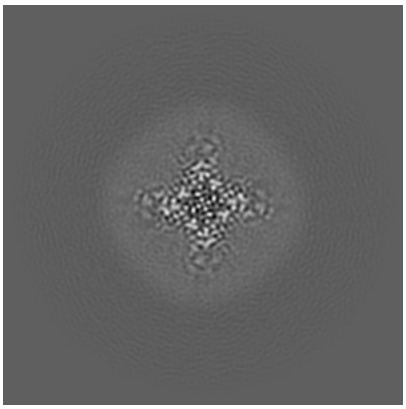
6.3.1 Primary map



X Index: 143

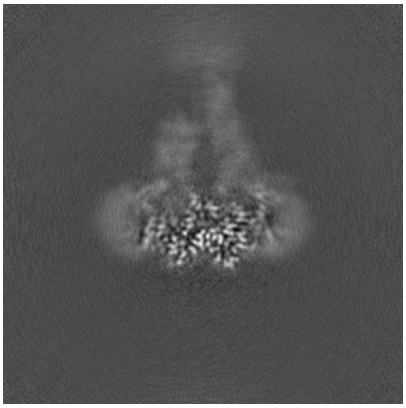


Y Index: 143

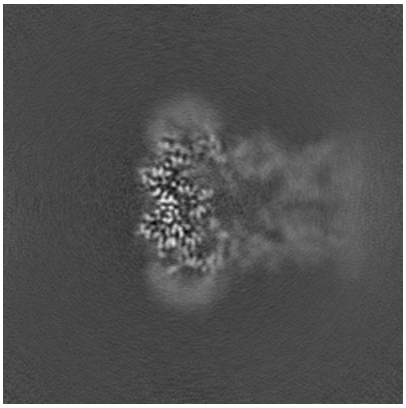


Z Index: 115

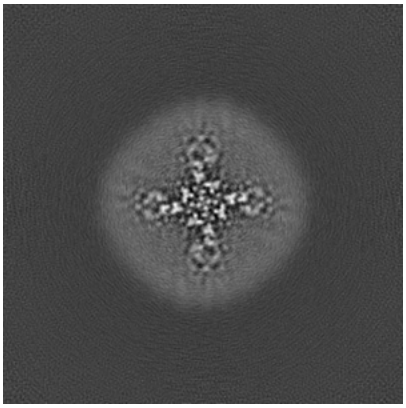
6.3.2 Raw map



X Index: 137



Y Index: 137

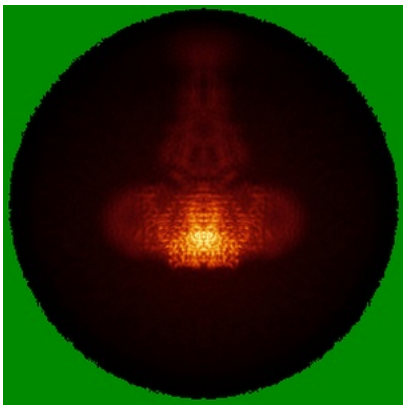


Z Index: 119

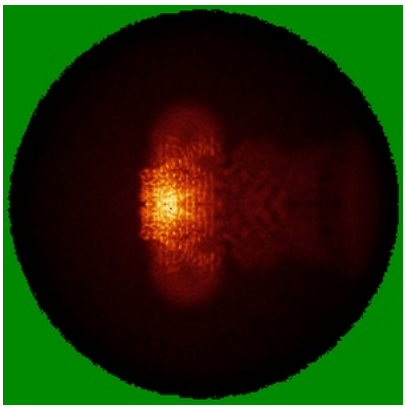
The images above show the largest variance slices of the map in three orthogonal directions.

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

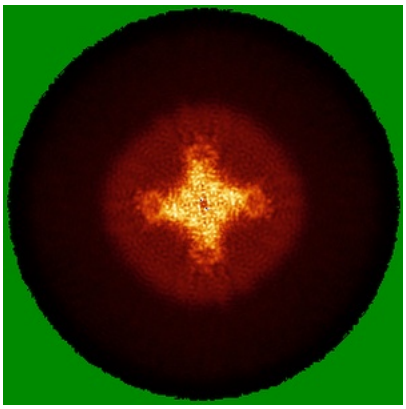
6.4.1 Primary map



X

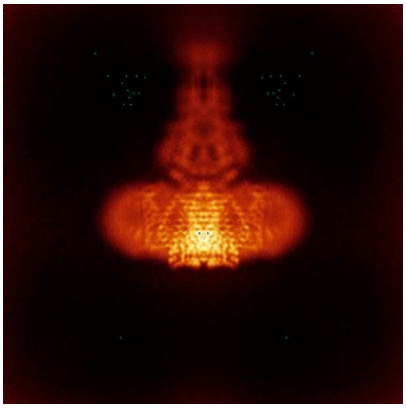


Y

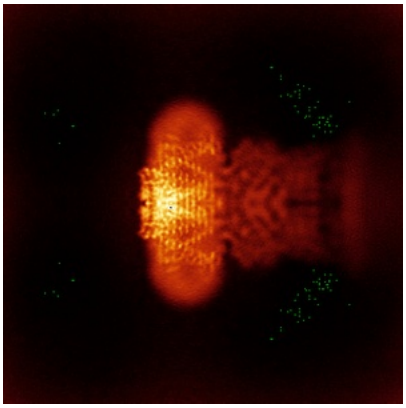


Z

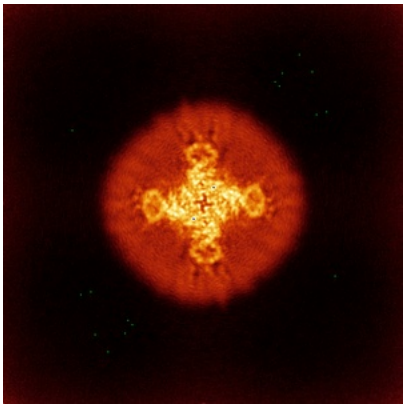
6.4.2 Raw map



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 0.184. 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.

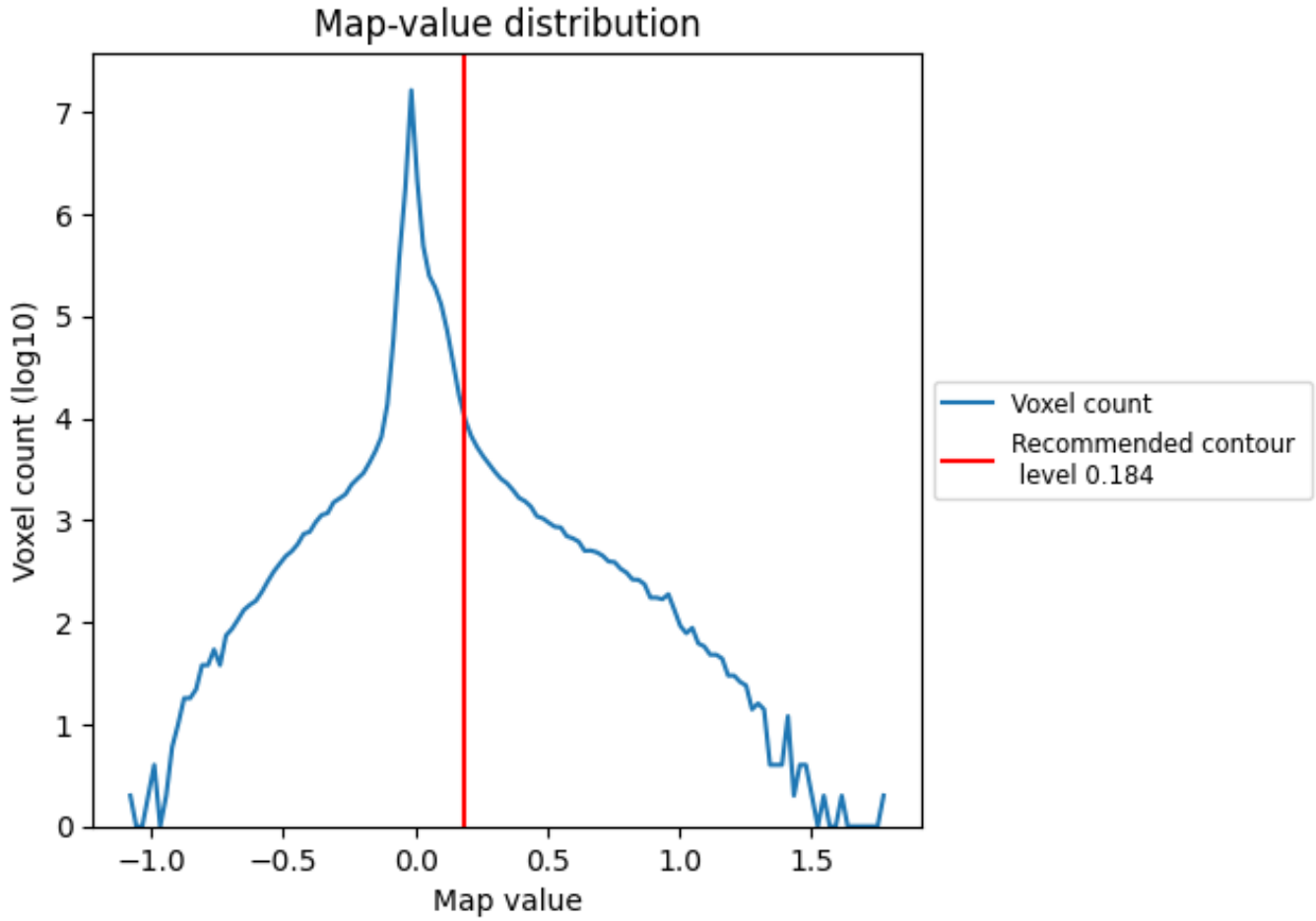
6.6 Mask visualisation (i)

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

7 Map analysis

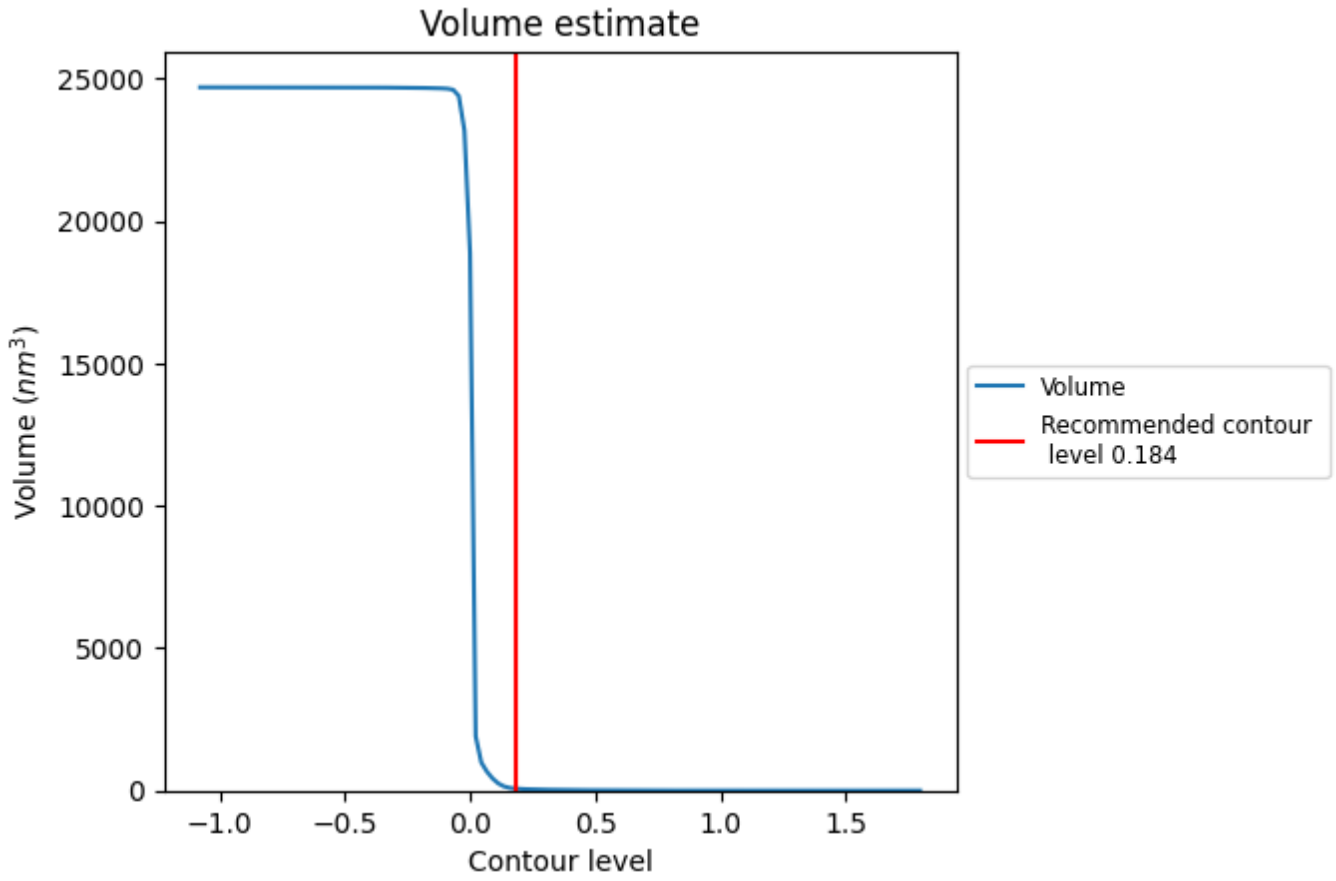
This section contains the results of statistical analysis of the map.

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.

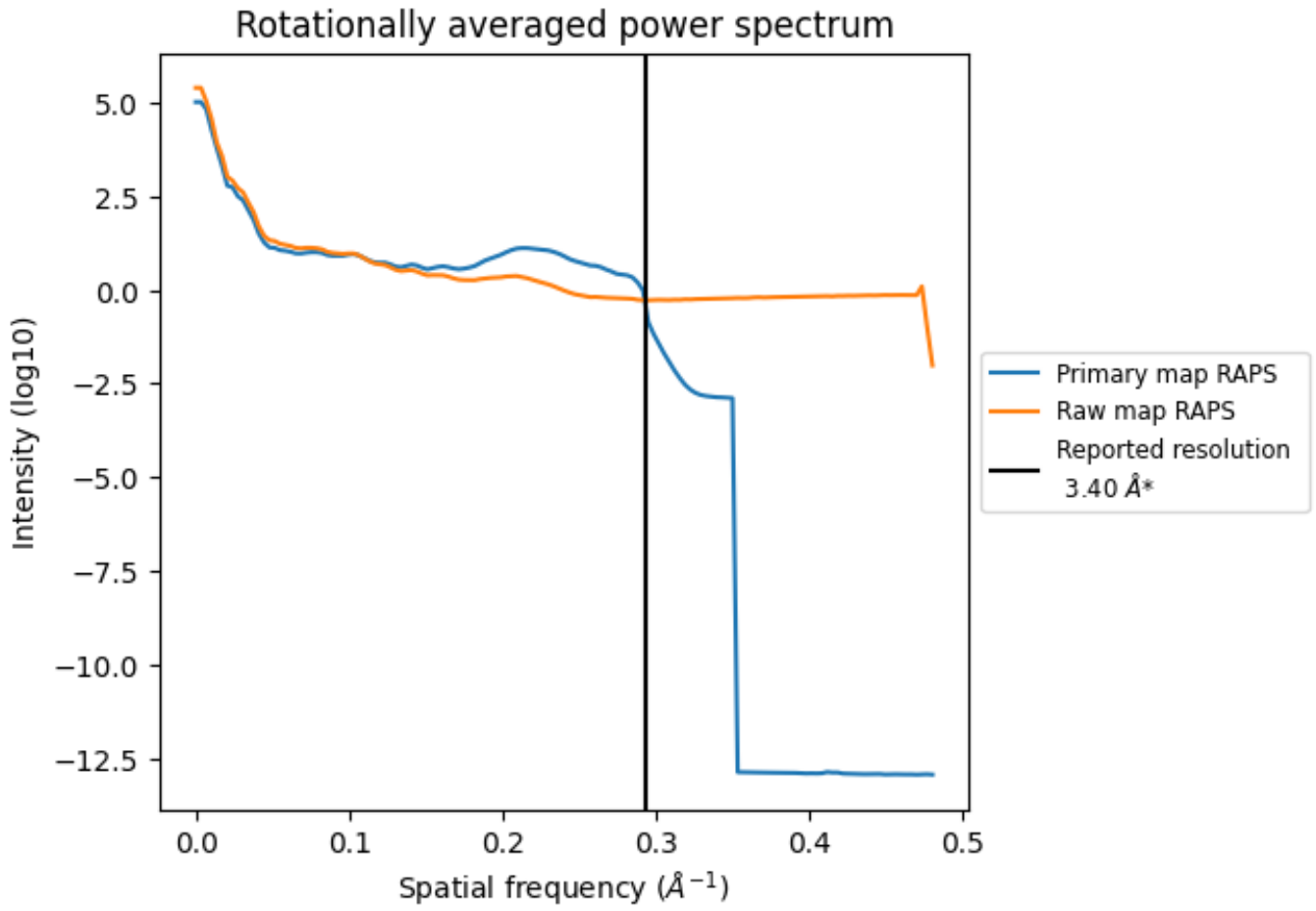
7.2 Volume estimate (i)



The volume at the recommended contour level is 67 nm^3; this corresponds to an approximate mass of 60 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)

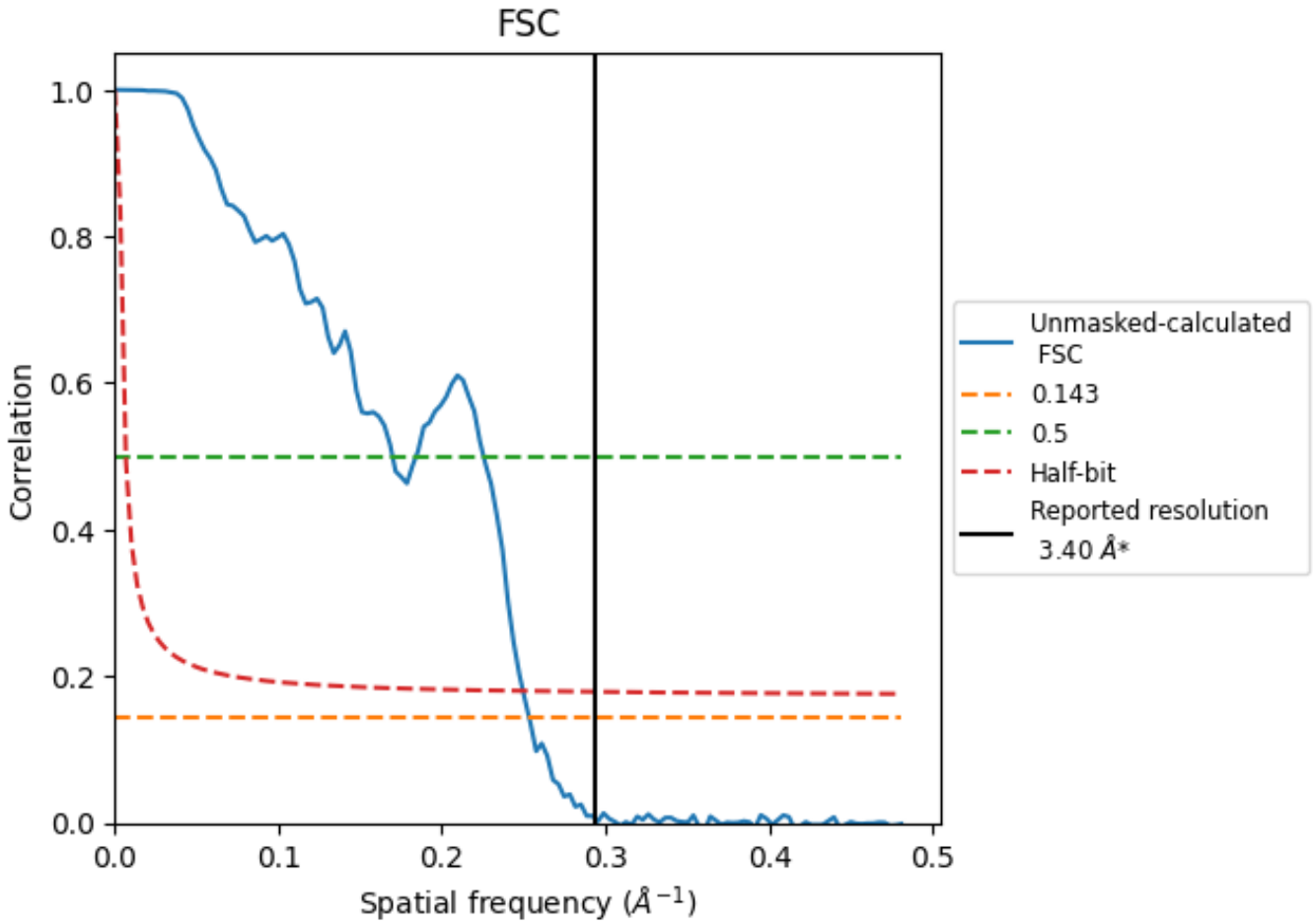


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

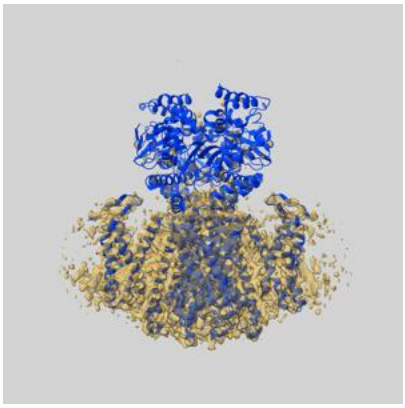
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.95	5.89	4.01

*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 3.95 differs from the reported value 3.4 by more than 10 %

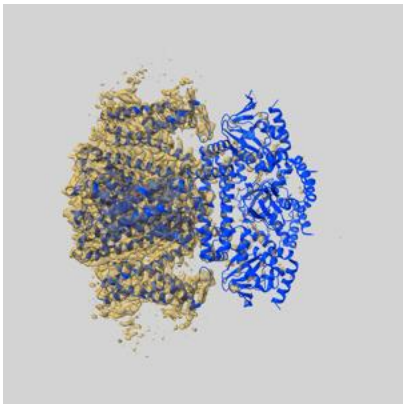
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-37855 and PDB model 8WUI. Per-residue inclusion information can be found in section 3 on page 6.

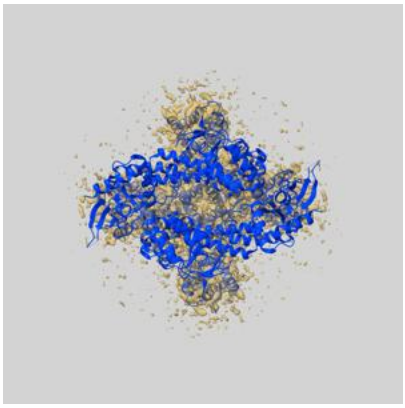
9.1 Map-model overlay



X



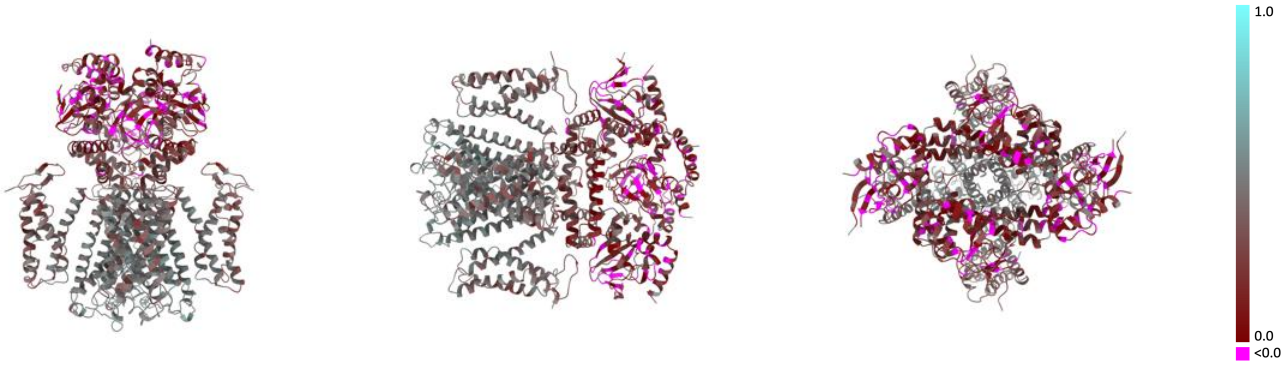
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.184 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.

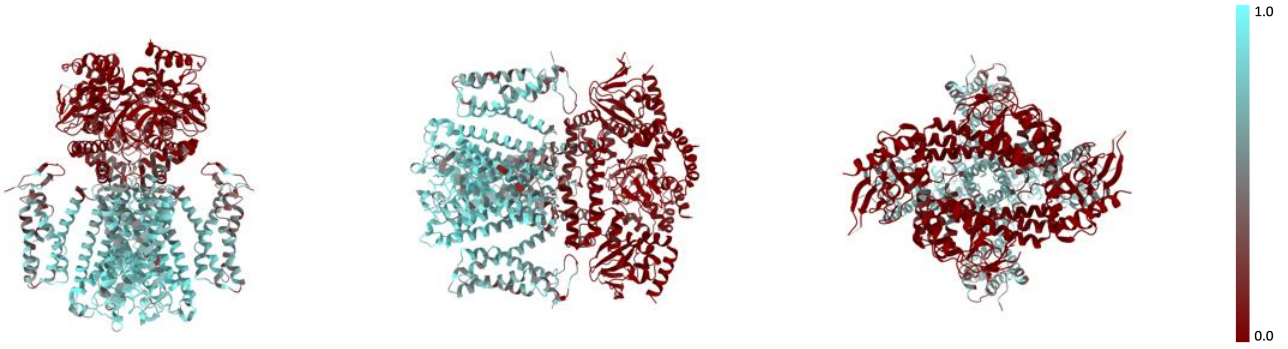
9.2 Q-score mapped to coordinate model



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.

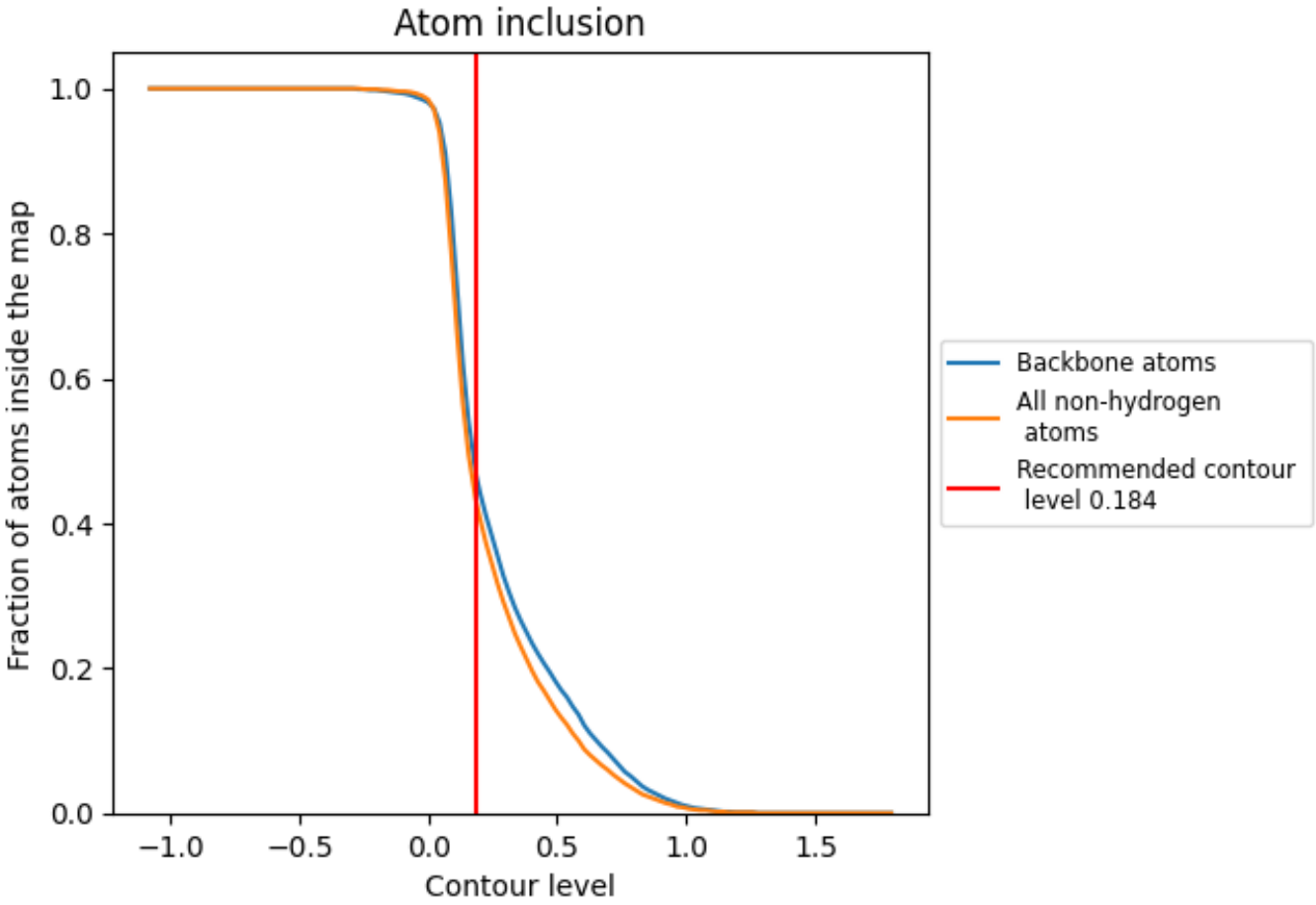
9.3 Atom inclusion mapped to coordinate model



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 (0.184).

9.4 Atom inclusion (i)



At the recommended contour level, 47% of all backbone atoms, 43% 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 (0.184) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4320	0.3320
A	0.4370	0.3420
B	0.4290	0.3350
C	0.4310	0.3280
D	0.4290	0.3220