wwPDB EM Validation Summary Report (i)

Dec 11, 2022 – 05:47 pm GMT

PDB ID	:	6SYT
EMDB ID	:	EMD-10347
Title	:	Structure of the SMG1-SMG8-SMG9 complex
Authors	:	Gat, Y.; Schuller, J.M.; Conti, E.
Deposited on	:	2019-10-01
Resolution	:	3.45 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:

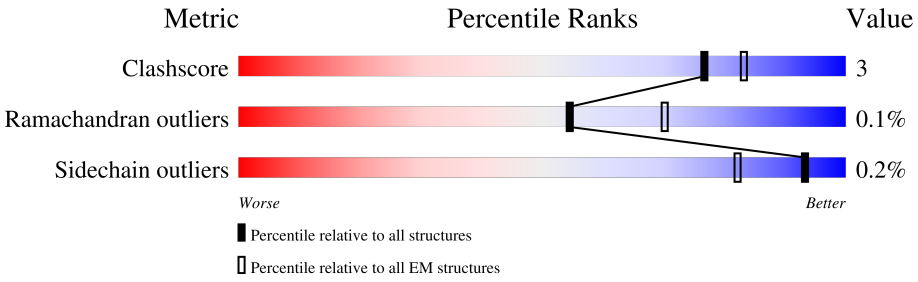
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.45 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	3712	12% 48% 49%
2	B	991	10% 35% 62%
3	C	520	54% 5% 41%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 18369 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 SMG1,Serine/threonine-protein kinase SMG1,SMG1,Serine/threonine-protein kinase SMG1,SMG1,Serine/threonine-protein kinase SMG1,SMG1,Serine/threonine-protein kinase SMG1,SMG1,Serine/threonine-protein kinase SMG1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1896	13209	8487	2365	2295	62	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	743	ARG	LYS	conflict	UNP Q96Q15
A	2335	ALA	ASP	engineered mutation	UNP Q96Q15

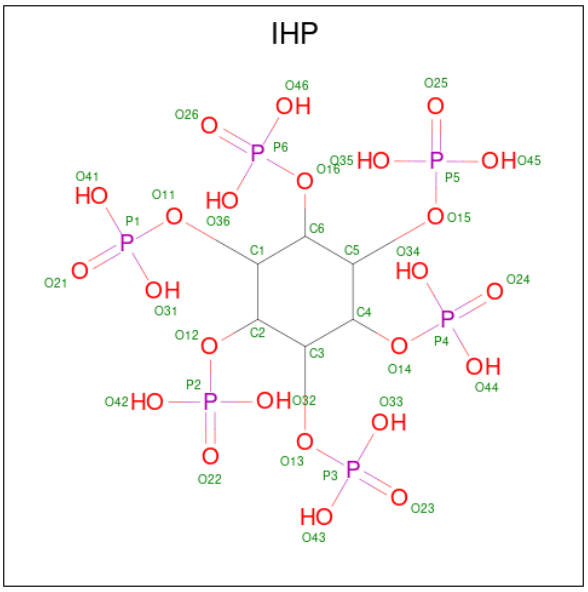
- Molecule 2 is a protein called Protein SMG8.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	377	2719	1772	487	447	13	0	0

- Molecule 3 is a protein called Protein SMG9.

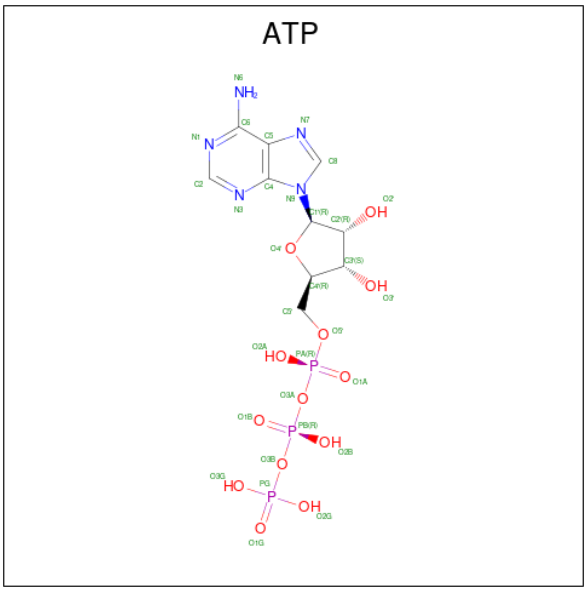
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	309	2373	1554	413	389	17	0	0

- Molecule 4 is INOSITOL HEXAKISPHOSPHATE (three-letter code: IHP) (formula: $C_6H_{18}O_{24}P_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	O	P	
4	A	1	36	6	24	6	0

- Molecule 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

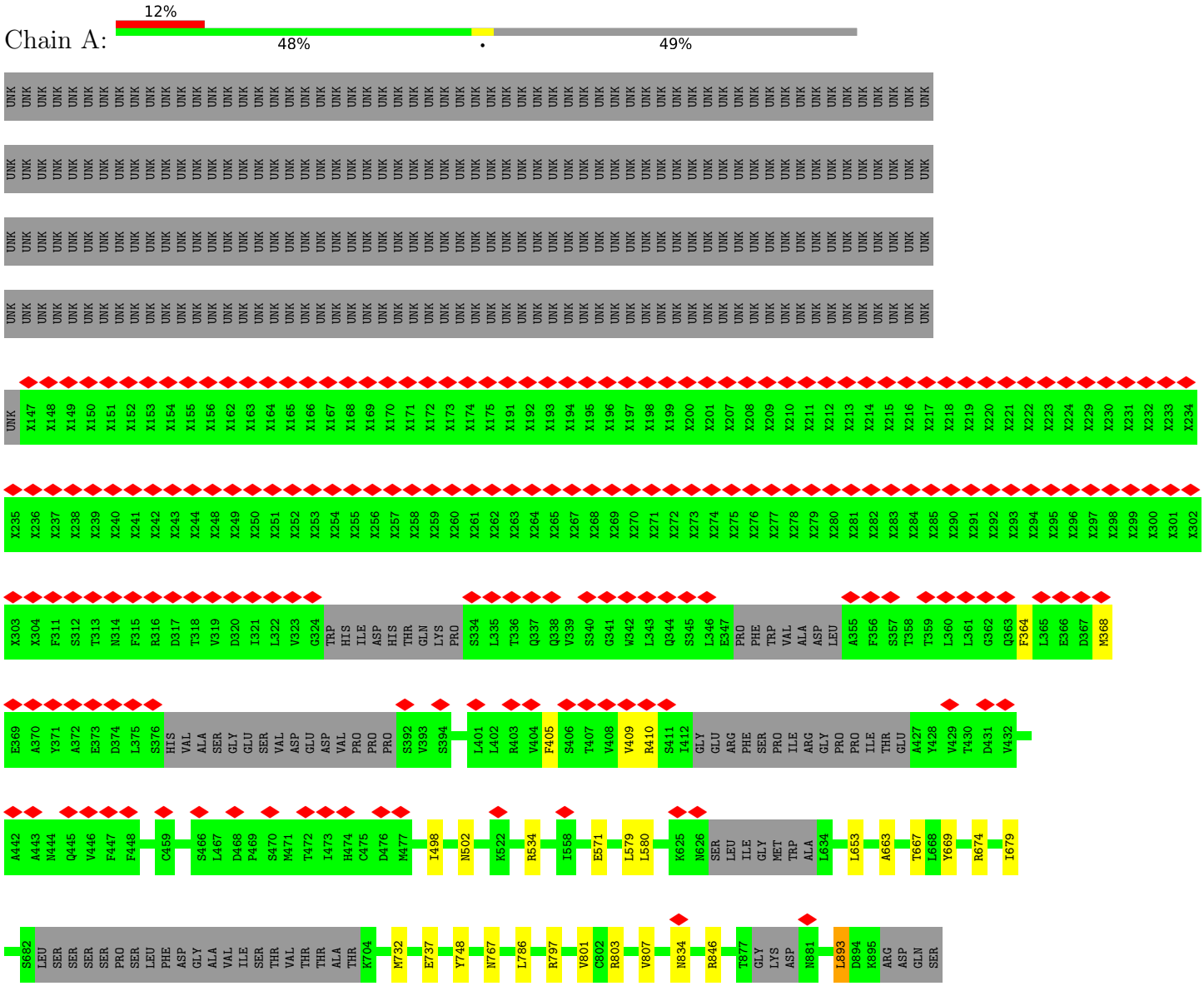
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	C	1	1	1	0

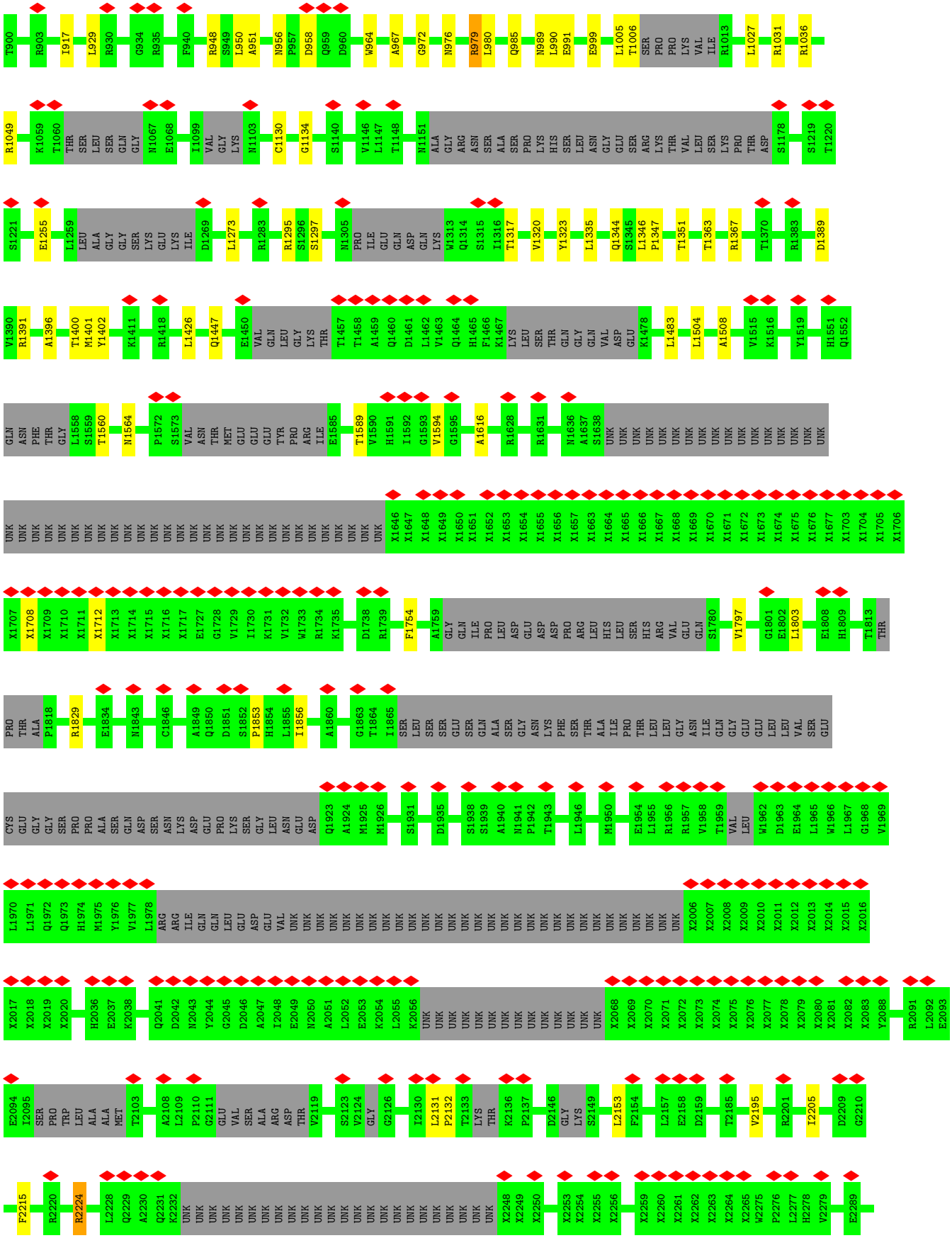
3 Residue-property plots (i)

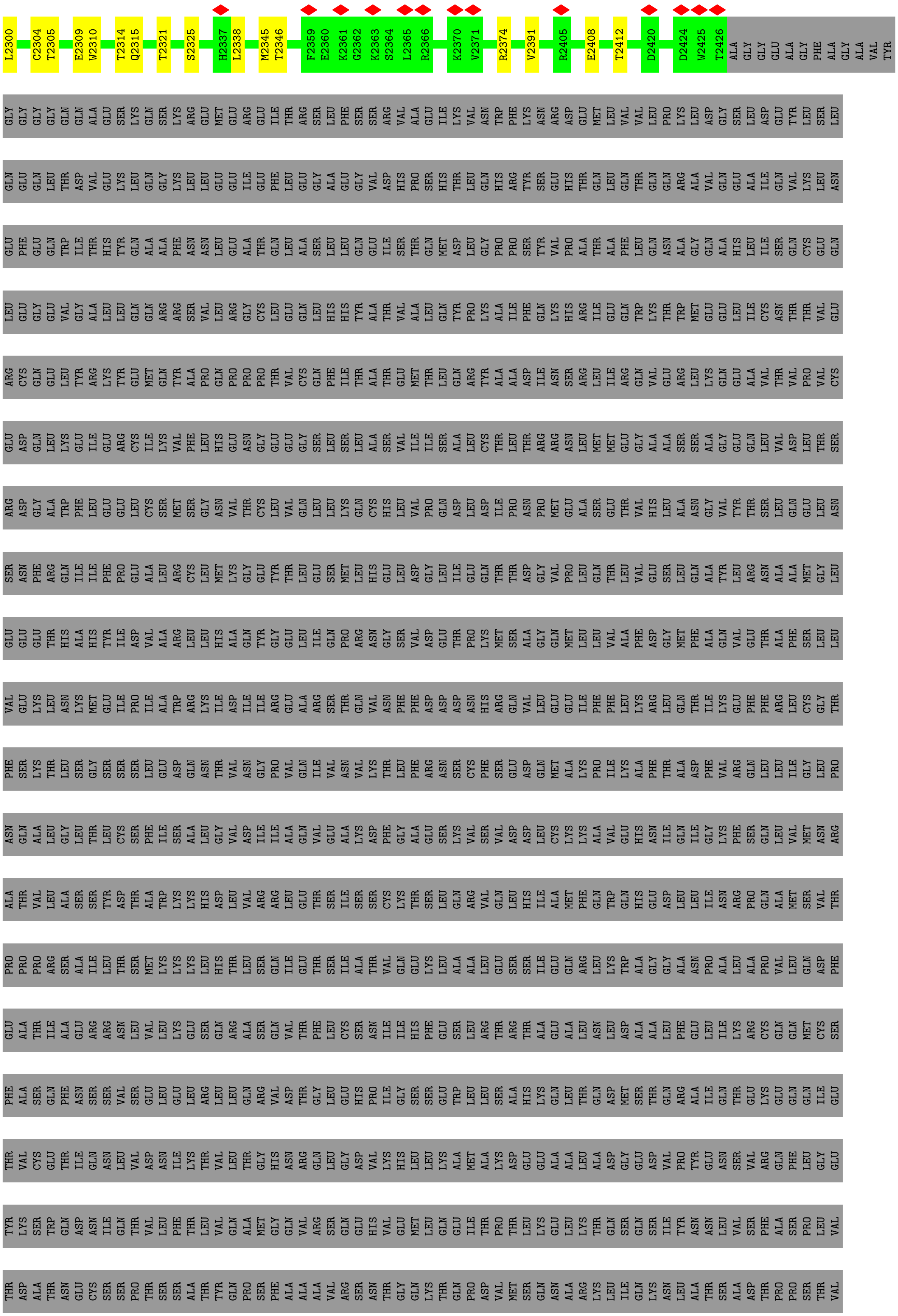
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

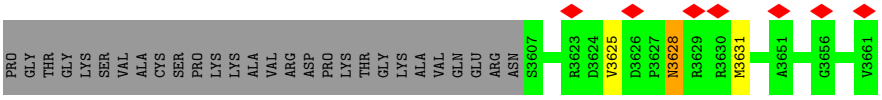
• Molecule 1: SMG1,Serine/threonine-protein kinase SMG1,SMG1,Serine/threonine-protein kinase SMG1,SMG1,Serine/threonine-protein kinase SMG1,SMG1,Serine/threonine-protein kinase SMG1,SMG1,Serine/threonine-protein kinase SMG1

Chain A:



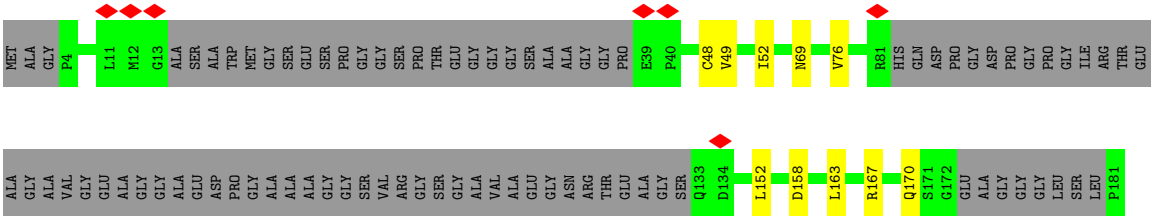


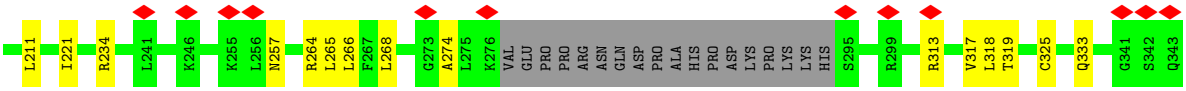

L2300 C2304 T2305 E2309 W2310 T2314 Q2315 T2321 S2325 H2337 L2338 M2345 T2346 F2359 E2360 K2361 G2362 K2363 S2364 L2365 R2366 K2370 V2371 R2374 V2391 R2405 E2408 T2412 D2420 D2424 W2425 T2426 ALA GLY GLY GLU ALA GLY PHE ALA GLY ALA VAL TYR
GLY GLY GLY GLY GLN GLN ALA GLU SER LYS GLN SER LYS ARG GLU MET GLU ARG GLU ILE THR ARG SER LEU PHE SER SER ARG VAL ALA GLU ILE LYS VAL ASN TRP PHE LYS ASN ARG ASP GLU MET LEU VAL VAL LEU PRO LYS LEU ASP GLY SER LEU ASP GLU TYR LEU SER LEU
GLN GLU GLN LEU THR ASP VAL GLU LYS LEU GLN GLY LYS LEU LEU GLU GLU ILE GLU PHE LEU GLU GLY ALA GLU GLY VAL ASP HIS PRO SER HIS THR LEU GLN HIS ARG TYR SER GLU HIS THR GLN LEU GLN THR GLN GLN ARG ALA VAL GLN GLU ALA ILE GLN VAL LYS LEU ASN
GLU PHE GLU GLN TRP ILE THR HIS TYR GLN ALA ALA PHE ASN ASN LEU GLU ALA THR GLN LEU ALA SER LEU LEU GLN GLU ILE SER THR GLN MET ASP LEU GLY PRO PRO SER TYR VAL PRO ALA THR ALA PHE LEU GLN ASN ALA GLY GLN ALA HIS LEU ILE SER GLN CYS GLU GLN
LEU GLU GLY GLU VAL GLY ALA LEU LEU GLN GLN ARG ARG SER VAL LEU ARG GLY CYS LEU GLU GLN LEU HIS HIS TYR ALA THR VAL ALA LEU GLN TYR PRO LYS ALA ILE PHE GLN LYS HIS ARG ILE GLU GLN TRP LYS THR TRP MET GLU GLU LEU ILE CYS ASN THR THR VAL GLU
ARG CYS GLN GLU LEU TYR ARG LYS TYR GLU MET GLN TYR ALA PRO GLN PRO PRO PRO THR VAL CYS GLN PHE ILE THR ALA THR GLU MET THR LEU GLN ARG TYR ALA ALA ASP ILE ASN SER ARG LEU ILE ARG GLN VAL GLU ARG LEU LYS GLN GLU ALA VAL THR VAL PRO VAL CYS
GLU ASP GLN LEU LYS GLU ILE GLU ARG CYS ILE LYS VAL PHE LEU HIS GLU ASN GLY GLU GLU GLY SER LEU SER LEU ALA SER VAL ILE ILE SER ALA LEU CYS THR LEU THR ARG ARG ASN LEU MET MET GLU GLY ALA ALA SER SER ALA GLY GLU GLN LEU VAL ASP LEU THR SER
ARG ASP GLY ALA TRP PHE LEU GLU GLU LEU CYS SER MET SER GLY ASN VAL THR CYS LEU VAL GLN LEU LEU LYS GLN CYS HIS LEU VAL PRO GLN ASP LEU ASP ILE PRO ASN PRO MET GLU ALA SER GLU THR VAL HIS LEU ALA ASN GLY VAL TYR THR SER LEU GLN GLU LEU ASN
SER ASN PHE ARG GLN ILE ILE PHE PRO GLU ALA LEU ARG CYS LEU MET LYS GLY GLU TYR THR LEU GLU SER MET LEU HIS GLU LEU ASP GLY LEU ILE GLU GLN THR THR ASP GLY VAL PRO LEU GLN THR LEU VAL GLU SER LEU GLN ALA TYR LEU ARG ASN ALA ALA MET GLY LEU
GLU GLU GLU THR HIS ALA HIS TYR ILE ASP VAL ALA ARG LEU LEU HIS ALA GLN TYR GLY GLU LEU ILE GLN PRO ARG ASN GLY SER VAL ASP GLU THR PRO LYS MET SER ALA GLY GLN MET LEU LEU VAL ALA PHE ASP GLY MET PHE ALA GLN VAL GLU THR ALA PHE SER LEU LEU
VAL GLU LYS LEU ASN LYS MET GLU ILE PRO ILE ALA TRP ARG LYS ILE ASP ILE ILE ARG GLU ALA ARG SER THR GLN VAL ASN PHE PHE ASP ASP ASN HIS ARG GLN VAL LEU GLU GLU ILE PHE PHE LEU LYS ARG LEU GLN THR ILE LYS GLU PHE PHE ARG LEU CYS GLY THR
PHE SER LYS THR LEU SER GLY SER SER SER LEU GLU ASP GLN ASN THR VAL ASN GLY PRO VAL GLN ILE VAL ASN VAL LYS THR LEU PHE ARG ASN SER CYS PHE SER GLU ASP GLN MET ALA LYS PRO ILE LYS ALA PHE THR ALA ASP PHE VAL ARG GLN LEU LEU ILE GLY LEU PRO
ASN GLN ALA LEU GLY LEU THR LEU CYS SER PHE ILE SER ALA LEU GLY VAL ASP ILE ILE ALA GLN VAL GLU ALA LYS ASP PHE GLY ALA GLU SER LYS VAL SER VAL ASP ASP LEU CYS LYS LYS ALA VAL GLU HIS ASN ILE GLN ILE GLY LYS PHE SER GLN LEU VAL MET ASN ARG
ALA THR VAL LEU ALA SER SER TYR ASP THR ALA TRP LYS LYS HIS ASP LEU VAL ARG ARG LEU GLU THR SER ILE SER SER CYS LYS THR SER LEU GLN ARG VAL GLN LEU HIS ILE ALA MET PHE GLN TRP GLN HIS GLU ASP SER LEU LEU ILE ASN ARG PRO GLN ALA MET SER VAL THR
PRO PRO PRO ARG SER ALA ILE LEU THR SER MET LYS LYS LYS LEU HIS THR LEU SER GLN ILE GLU THR SER ILE ALA THR VAL GLN GLU LYS LEU ALA ALA LEU GLU SER SER ILE GLU GLN ARG LEU LYS TRP ALA GLY GLY ALA ASN PRO ALA LEU ALA PRO VAL LEU GLN ASP PHE
GLU ALA THR ILE ALA GLU ARG ARG ASN LEU VAL LEU LYS GLU GLN SER GLN ARG ALA SER GLN VAL THR PHE LEU CYS SER ASN ILE ILE HIS PHE GLU SER LEU ARG THR ARG THR ALA GLU ALA LEU ASN LEU ASP ALA ALA LEU PHE GLU LEU ILE LYS ARG CYS GLN GLN MET CYS SER
PHE ALA SER GLN PHE ASN SER SER VAL SER GLU LEU GLU LEU ARG LEU LEU GLN ARG VAL ASP THR GLY LEU GLU HIS PRO ILE GLY SER SER GLU TRP LEU LEU SER ALA HIS LYS GLN LEU THR GLN ASP MET SER THR GLN ARG ALA ILE GLN THR GLU LYS GLU GLN GLN ILE GLU
THR VAL CYS GLU THR ILE GLN ASN LEU VAL ASP ASN ILE LYS THR VAL LEU THR GLY HIS ASN ARG GLN LEU GLY ASP VAL LYS HIS LEU LEU LYS ALA MET ALA LYS ASP GLU GLU ALA ALA LEU ALA ASP GLY GLU ASP VAL PRO TYR GLU ASN SER VAL ARG GLN PHE LEU GLY GLU
TYR LYS SER TRP GLN ASP ASN ILE GLN THR VAL LEU PHE THR LEU VAL GLN ALA MET GLY GLN VAL ARG SER GLN GLU HIS VAL GLU MET LEU GLN GLU ILE THR PRO THR LEU LYS GLU LEU LYS THR GLN SER GLN SER ILE TYR ASN ASN LEU VAL SER PHE ALA SER PRO LEU VAL
THR ASP ALA THR ASN GLU CYS SER SER PRO THR SER SER ALA THR TYR GLN PRO SER PHE ALA ALA ALA VAL ARG SER ASN THR GLY GLN LYS THR GLN PRO ASP VAL MET SER GLN ASN ALA ARG LYS LEU ILE GLN LYS ASN LEU ALA THR SER ALA ASP THR PRO PRO SER THR VAL

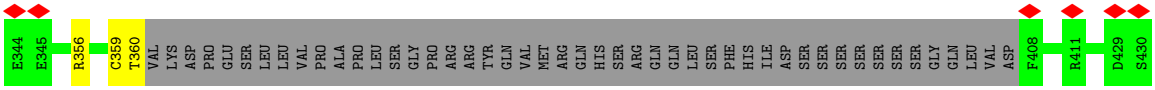


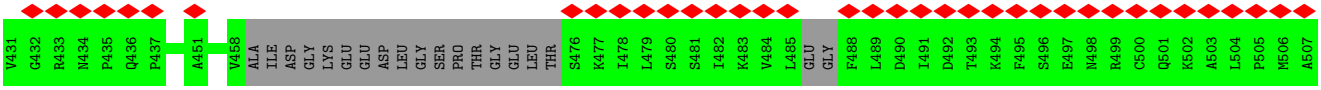
• Molecule 2: Protein SMG8

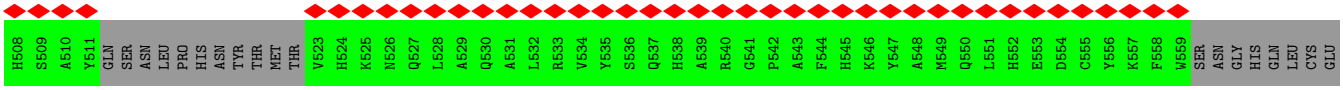
Chain B:

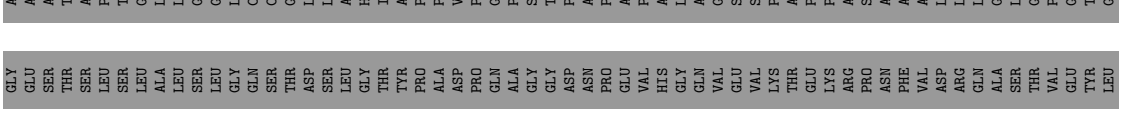


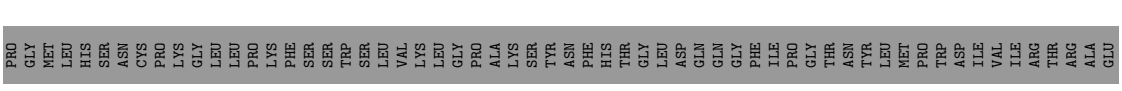


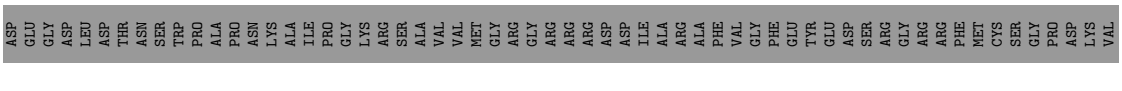


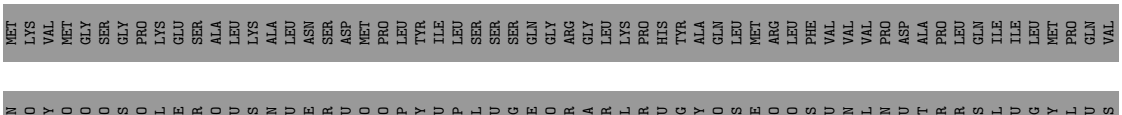






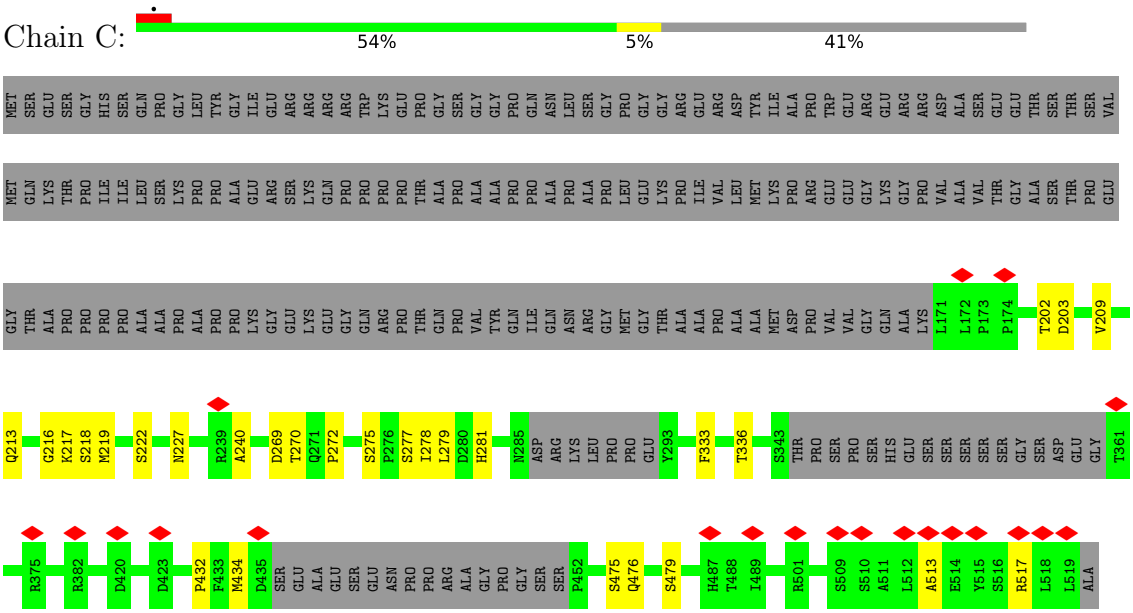






• Molecule 3: Protein SMG9

Chain C:


54%
5%
41%
MET SER GLU SER GLY HIS SER GLN PRO GLY LEU TYR GLY ILE GLU ARG ARG ARG ARG TRP LYS GLU PRO GLY SER GLY GLY PRO GLN ASN LEU SER GLY PRO GLY GLY ARG GLU ARG ASP TYR ILE ALA PRO TRP GLU ARG GLU ARG ARG ASP ALA SER GLU GLU THR SER THR SER VAL
MET GLN LYS THR PRO ILE ILE LEU SER LYS PRO PRO ALA GLU ARG SER LYS GLN PRO PRO PRO THR ALA PRO ALA ALA PRO PRO ALA PRO ALA PRO PRO LEU GLU LYS PRO ILE VAL LEU MET LYS PRO ARG GLU GLU GLY LYS GLY PRO VAL ALA VAL THR GLY ALA SER THR PRO GLU
GLY THR ALA PRO PRO PRO PRO ALA ALA ALA PRO ALA ALA PRO PRO LYS GLY GLU LYS GLU GLY GLN ARG PRO THR GLN PRO VAL TYR GLN ILE GLN ASN ARG GLY MET GLY THR ALA ALA PRO ALA ALA MET ASP PRO VAL VAL GLY GLN ALA LYS L171 L172 P173 P174 T202 D203 V209
Q213 G216 K217 S218 M219 S322 N227 R239 A240 D269 T270 Q271 P272 S275 P276 S277 I278 L279 D280 H281 N285 ASP ARG LYS LEU PRO PRO GLU Y293 F333 T336 S343 THR PRO SER PRO SER HIS GLU SER SER SER SER GLY SER ASP GLU GLY T361
R375 R382 D420 D423 P432 F433 M434 D435 SER GLU ALA GLU SER GLU ASN PRO PRO ARG ALA GLY PRO GLY SER SER P452 S475 Q476 S479 H487 T488 I489 R501 S509 S510 A511 L512 A513 E514 Y515 S516 R517 L518 L519 ALA

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	214254	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 ($e^-/Å^2$)	52.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.381	Depositor
Minimum map value	-0.234	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.07	Depositor
Map size (Å)	317.99997, 317.99997, 317.99997	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.76	0/12363	0.67	7/16876 (0.0%)
2	B	0.67	0/2777	0.69	1/3783 (0.0%)
3	C	0.94	0/2433	0.75	0/3308
All	All	0.77	0/17573	0.69	8/23967 (0.0%)

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	893	LEU	CB-CG-CD2	7.66	124.03	111.00
1	A	803	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	A	979	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	A	579	LEU	CA-CB-CG	5.34	127.58	115.30
1	A	948	ARG	NE-CZ-NH2	-5.33	117.64	120.30

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	13209	0	11704	65	0
2	B	2719	0	2502	18	0
3	C	2373	0	2311	22	0

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Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	36	0	4	1	0
5	C	31	0	12	8	0
6	C	1	0	0	0	0
All	All	18369	0	16533	103	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 3.

The worst 5 of 103 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:846:ARG:NH2	1:A:2309:GLU:OE2	2.10	0.84
1:A:964:TRP:HZ2	1:A:980:LEU:HD13	1.42	0.84
3:C:272:PRO:HG3	5:C:601:ATP:O3G	1.81	0.81
3:C:218:SER:OG	3:C:269:ASP:OD2	2.00	0.80
1:A:1297:SER:O	1:A:1402:TYR:OH	2.01	0.78

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	1617/3712 (44%)	1507 (93%)	109 (7%)	1 (0%)	51 84
2	B	359/991 (36%)	328 (91%)	30 (8%)	1 (0%)	41 75
3	C	301/520 (58%)	269 (89%)	32 (11%)	0	100 100
All	All	2277/5223 (44%)	2104 (92%)	171 (8%)	2 (0%)	54 84

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3628	ASN
2	B	274	ALA

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	1114/2768 (40%)	1112 (100%)	2 (0%)	93 98
2	B	238/847 (28%)	237 (100%)	1 (0%)	91 97
3	C	238/450 (53%)	238 (100%)	0	100 100
All	All	1590/4065 (39%)	1587 (100%)	3 (0%)	93 98

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	786	LEU
1	A	3628	ASN
2	B	170	GLN

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	546	HIS
1	A	1564	ASN
3	C	252	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)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\#\|Z\| > 2$
5	ATP	C	601	6	26,33,33	0.66	0	31,52,52	0.72	1 (3%)
4	IHP	A	3701	-	36,36,36	1.47	6 (16%)	54,60,60	2.00	9 (16%)

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
5	ATP	C	601	6	-	4/18/38/38	0/3/3/3
4	IHP	A	3701	-	-	5/30/54/54	0/1/1/1

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	3701	IHP	P5-O15	3.20	1.65	1.59
4	A	3701	IHP	P6-O16	3.09	1.65	1.59
4	A	3701	IHP	P4-O14	3.05	1.65	1.59
4	A	3701	IHP	P3-O13	2.85	1.64	1.59
4	A	3701	IHP	P1-O11	2.75	1.64	1.59

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	3701	IHP	O14-C4-C5	6.01	122.85	108.69

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	3701	IHP	O15-C5-C4	5.39	121.40	108.69
4	A	3701	IHP	C4-C3-C2	5.22	121.84	110.41
4	A	3701	IHP	O15-C5-C6	5.21	120.97	108.69
4	A	3701	IHP	O13-C3-C2	4.91	120.26	108.69

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	3701	IHP	C5-C4-O14-P4
4	A	3701	IHP	C6-C5-O15-P5
5	C	601	ATP	O4'-C4'-C5'-O5'
4	A	3701	IHP	C1-O11-P1-O21
4	A	3701	IHP	C2-C3-O13-P3

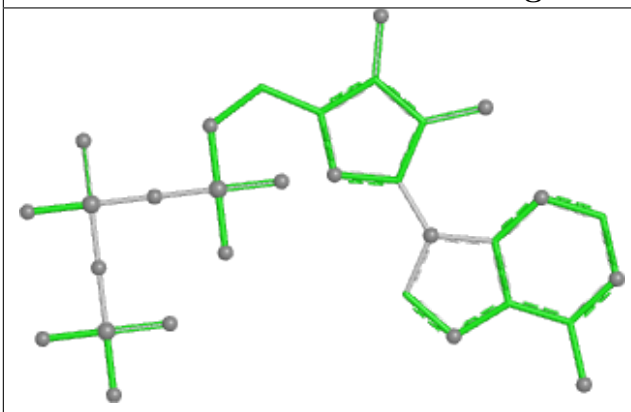
There are no ring outliers.

2 monomers are involved in 9 short contacts:

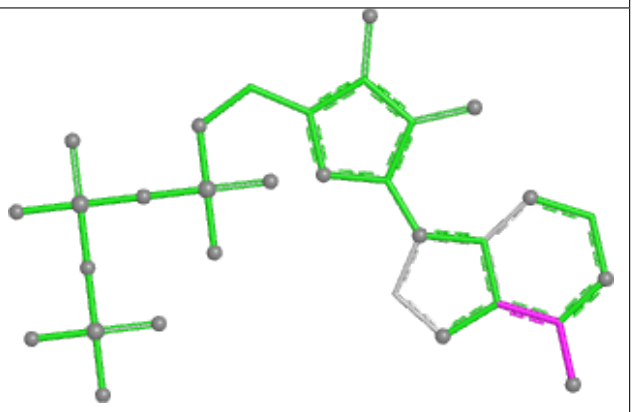
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	601	ATP	8	0
4	A	3701	IHP	1	0

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.

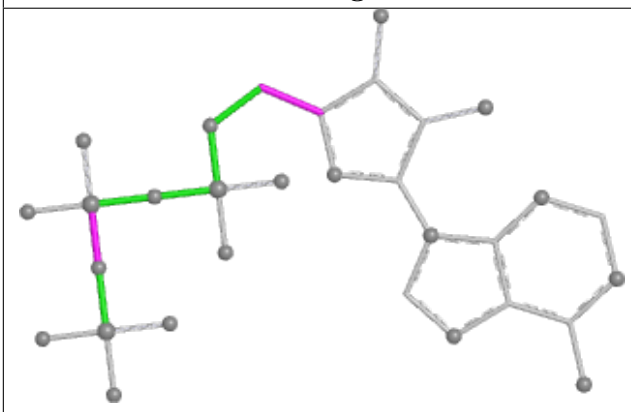
Ligand ATP C 601



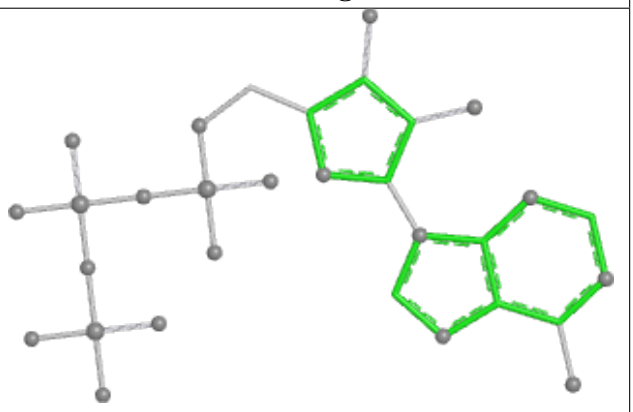
Bond lengths



Bond angles

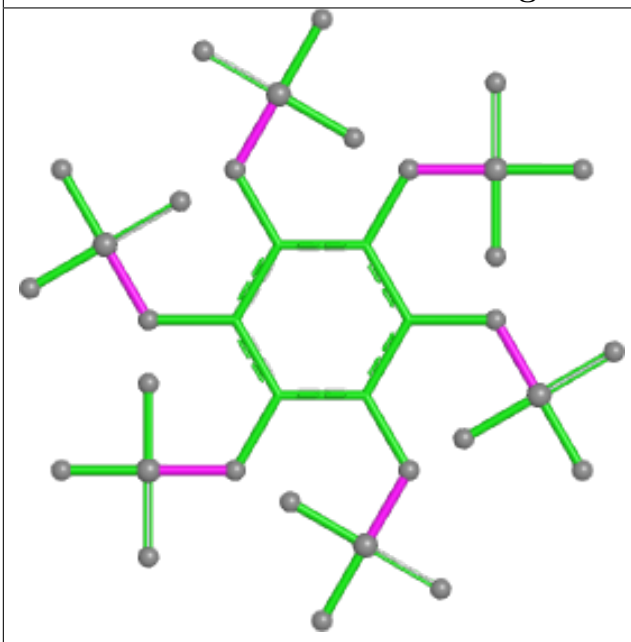


Torsions

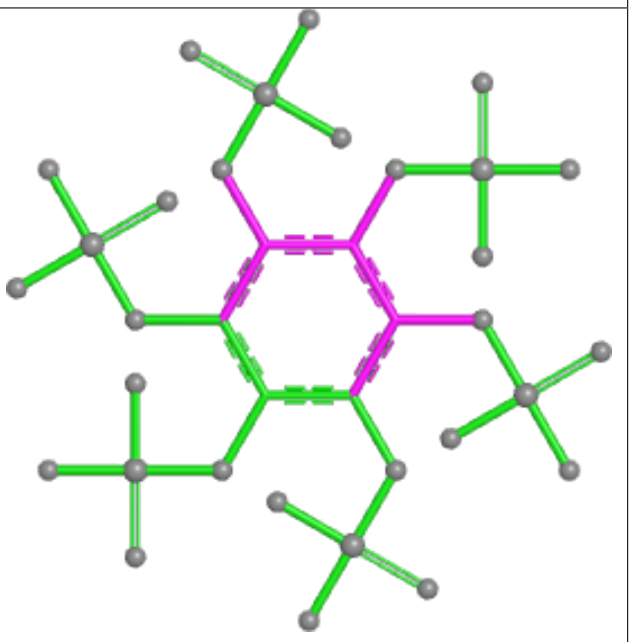


Rings

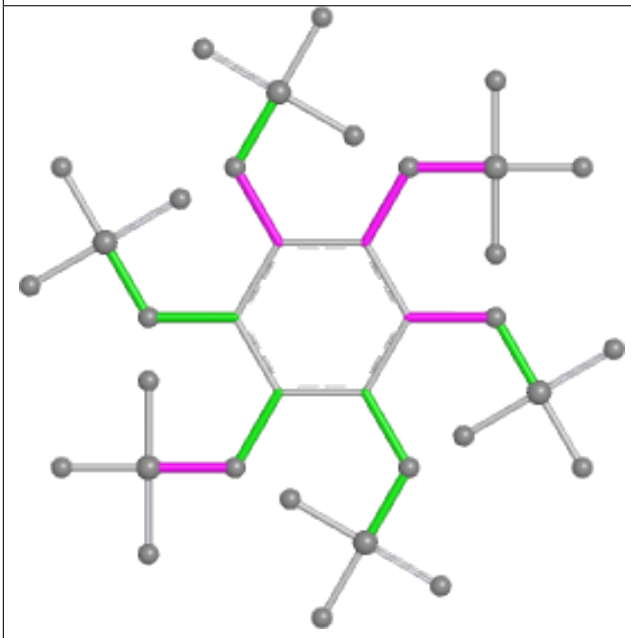
Ligand IHP A 3701



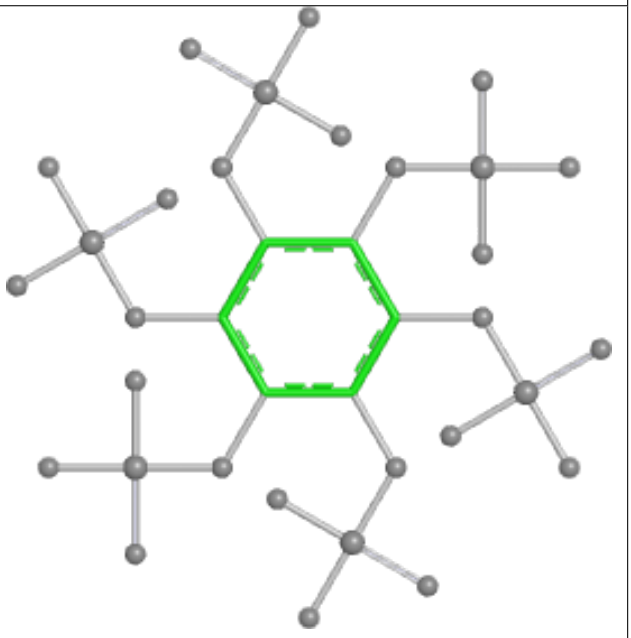
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	14

The worst 5 of 14 chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1717:UNK	C	1727:GLU	N	16.23
1	A	1677:UNK	C	1703:UNK	N	13.65
1	A	175:UNK	C	191:UNK	N	13.07
1	A	2021:UNK	C	2035:PRO	N	12.55
1	A	304:UNK	C	311:PHE	N	12.30

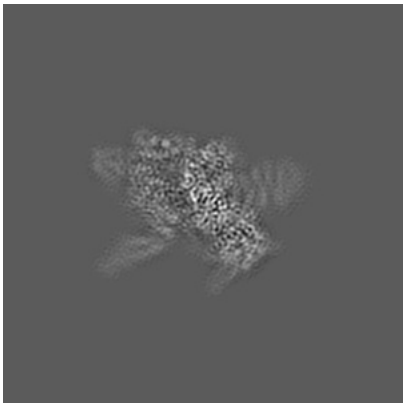
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-10347. These allow visual inspection of the internal detail of the map and identification of artifacts.

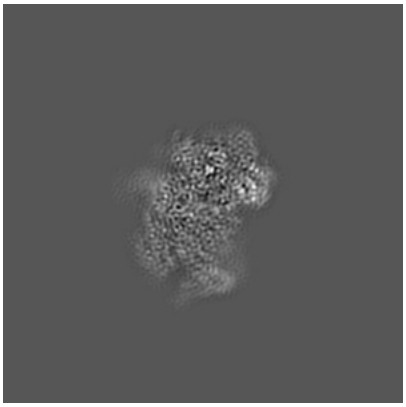
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

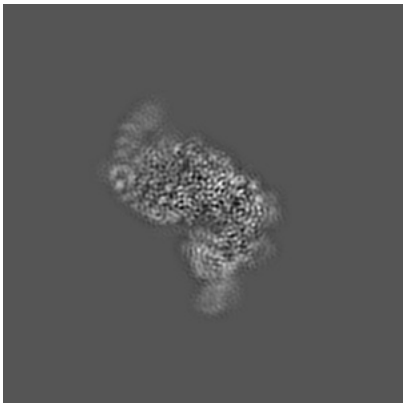
6.1.1 Primary map



X



Y

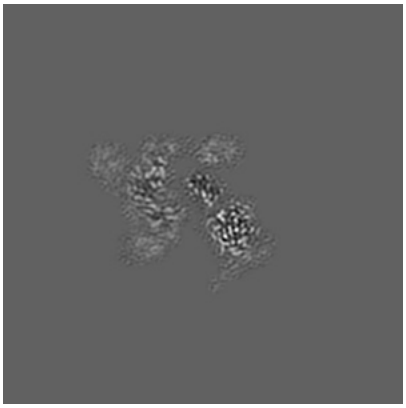


Z

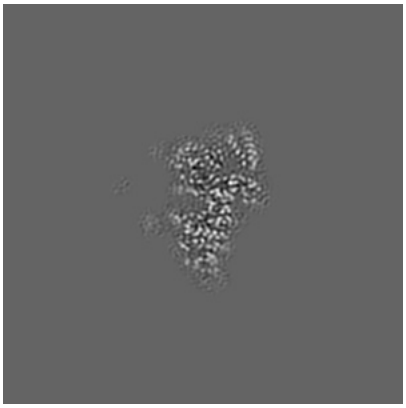
The images above show the map projected in three orthogonal directions.

6.2 Central slices

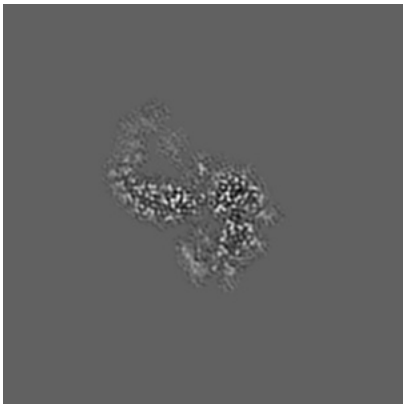
6.2.1 Primary map



X Index: 150



Y Index: 150

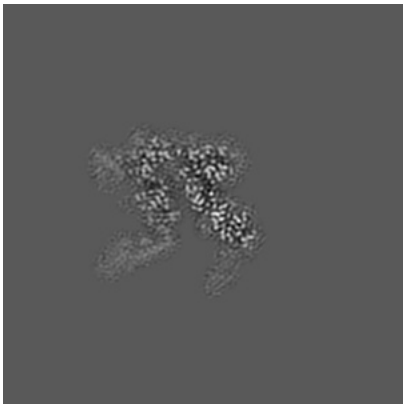


Z Index: 150

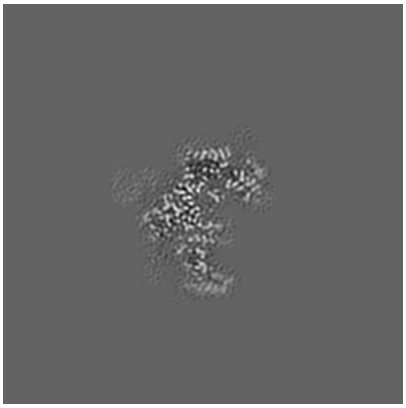
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 162



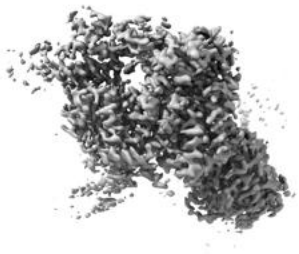
Y Index: 162

Z Index: 160

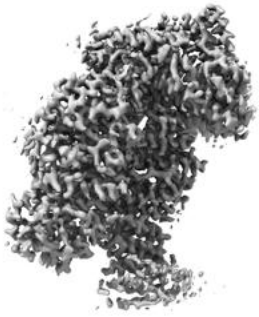
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.07. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

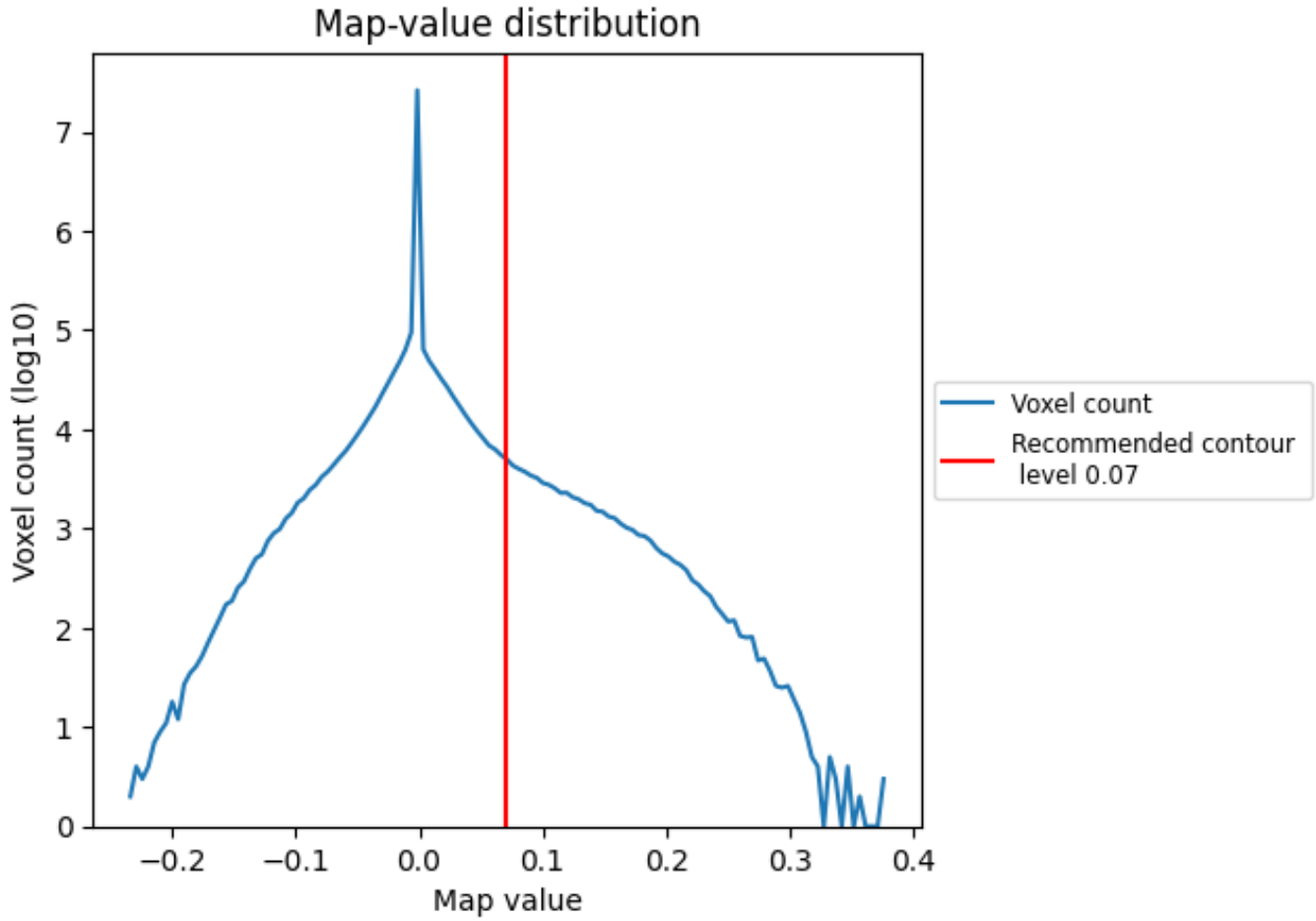
6.5 Mask visualisation (i)

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

7 Map analysis

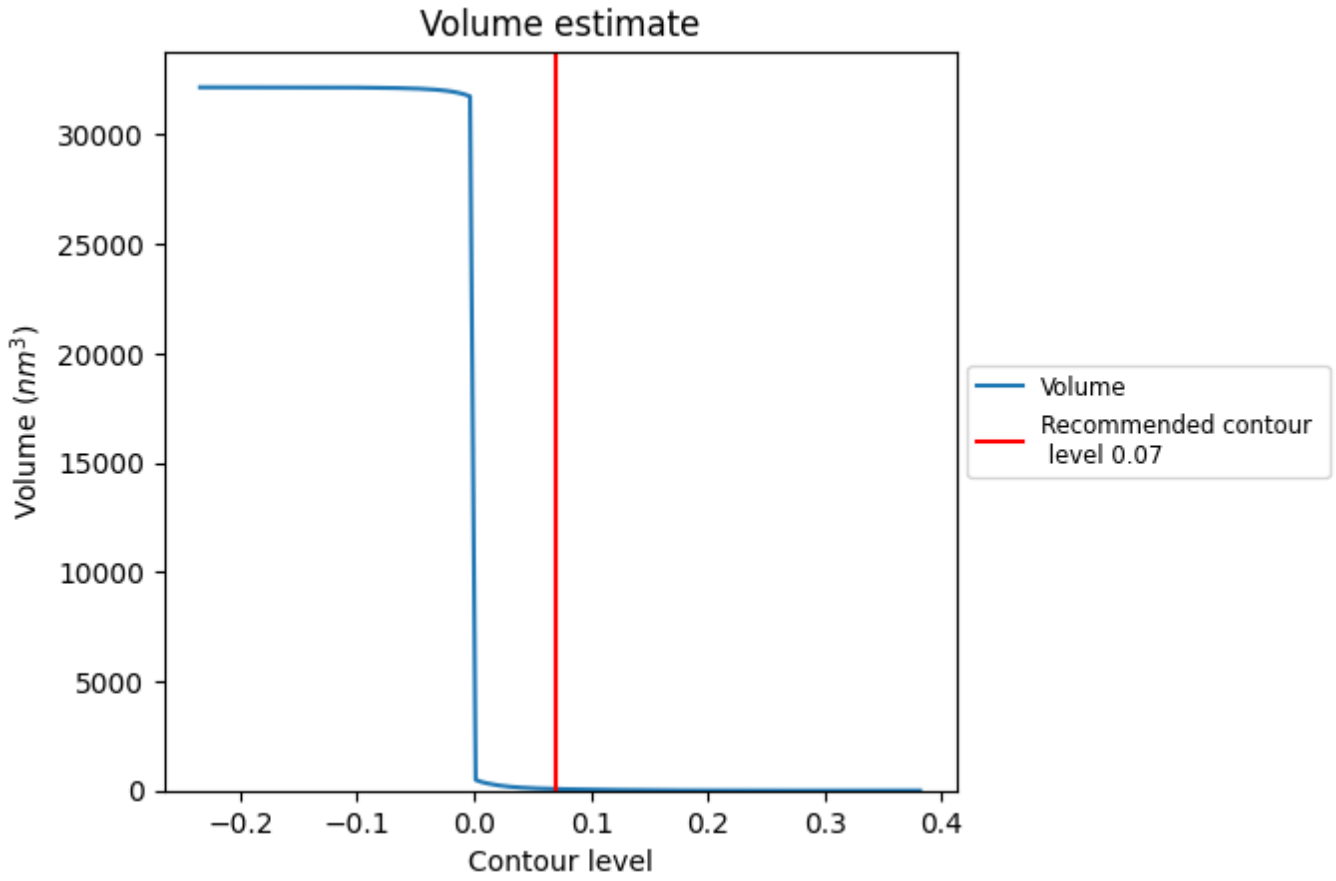
This section contains the results of statistical analysis of the map.

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.

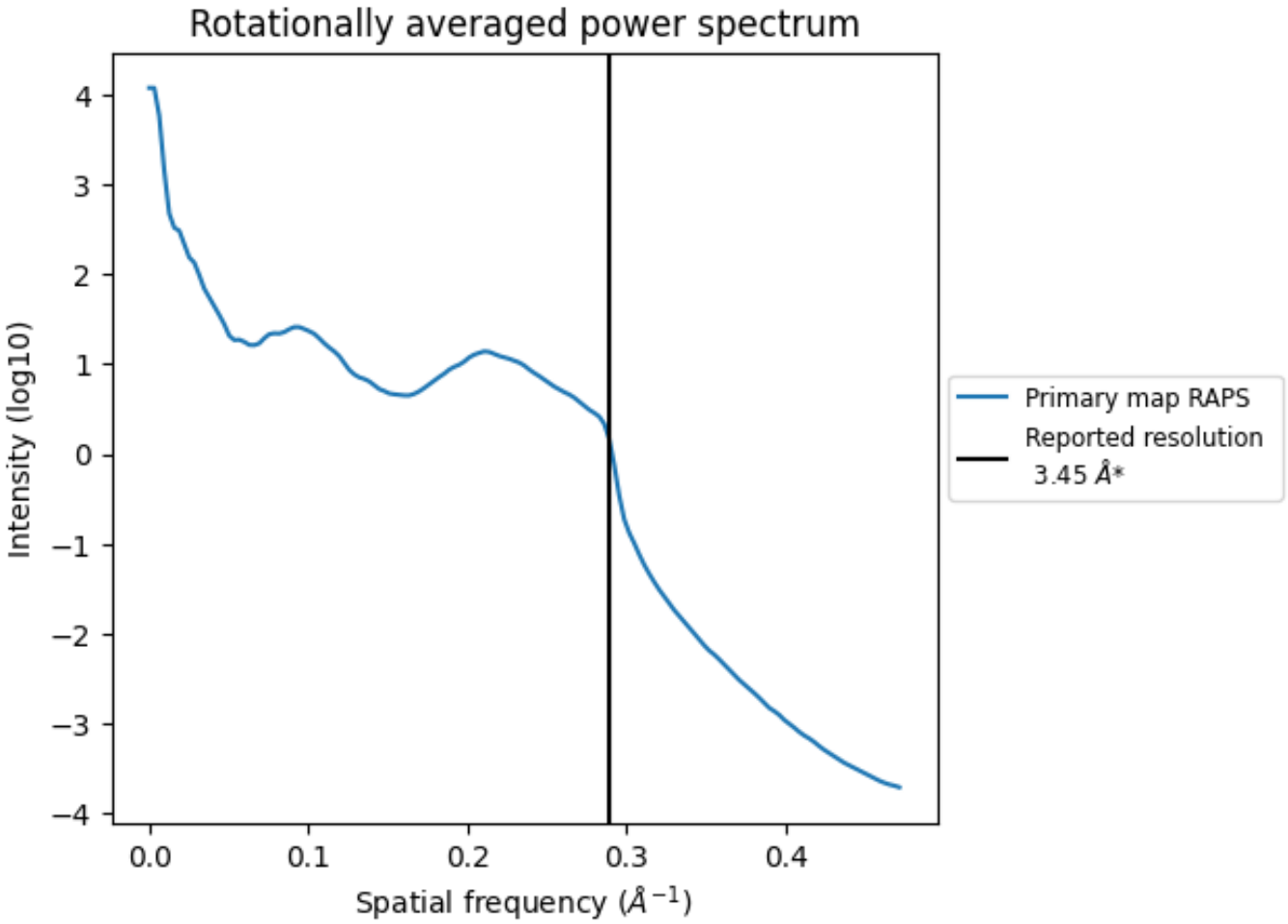
7.2 Volume estimate (i)



The volume at the recommended contour level is 74 nm^3; this corresponds to an approximate mass of 66 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 0.290 Å^{-1}

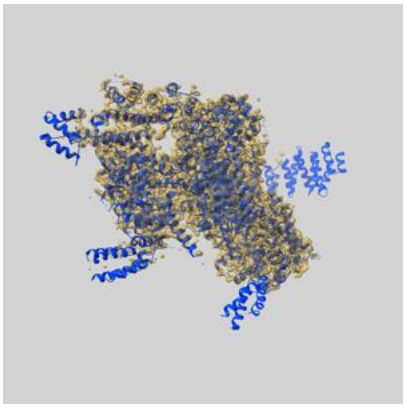
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

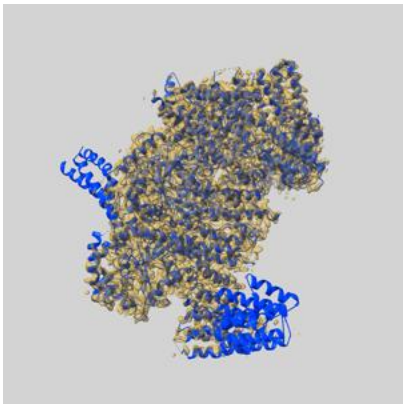
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-10347 and PDB model 6SYT. Per-residue inclusion information can be found in section 3 on page 6.

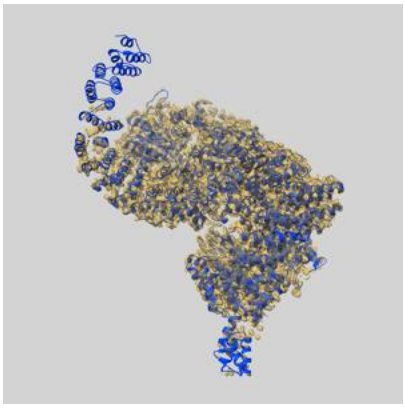
9.1 Map-model overlay



X



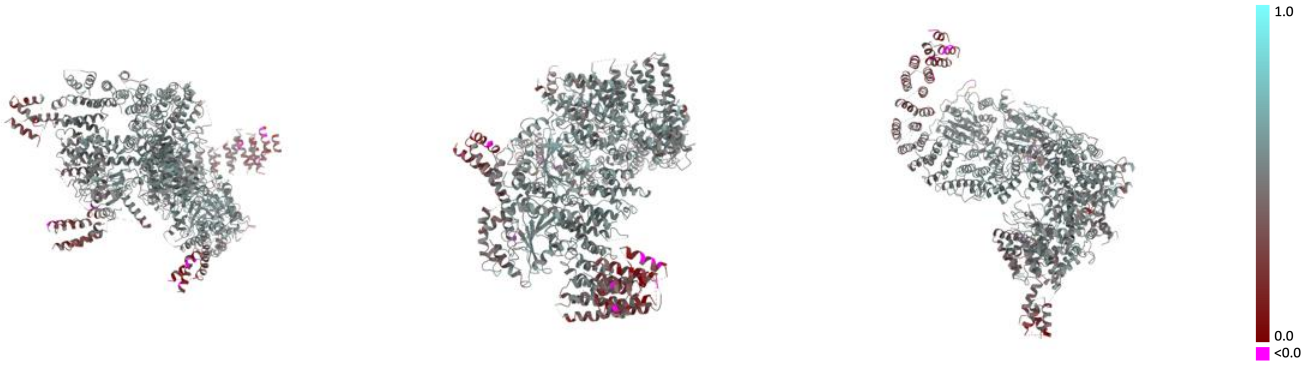
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.07 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.

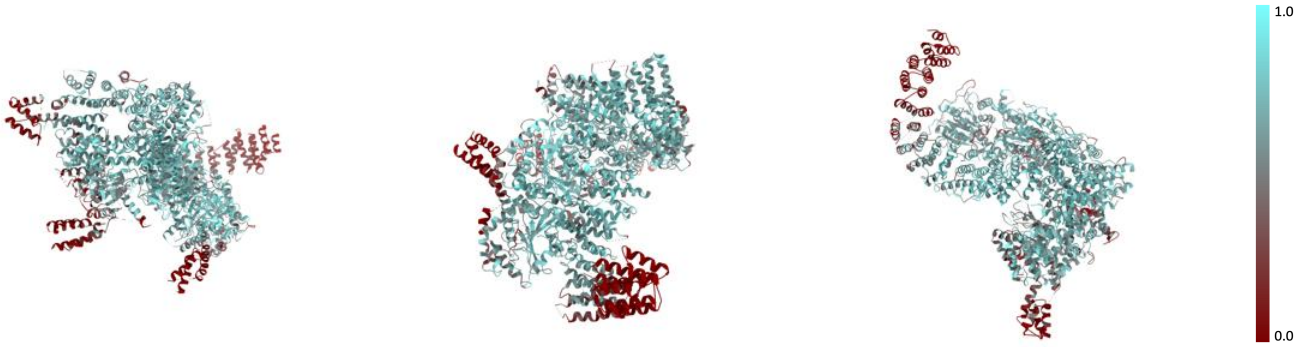
9.2 Q-score mapped to coordinate model (i)



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.

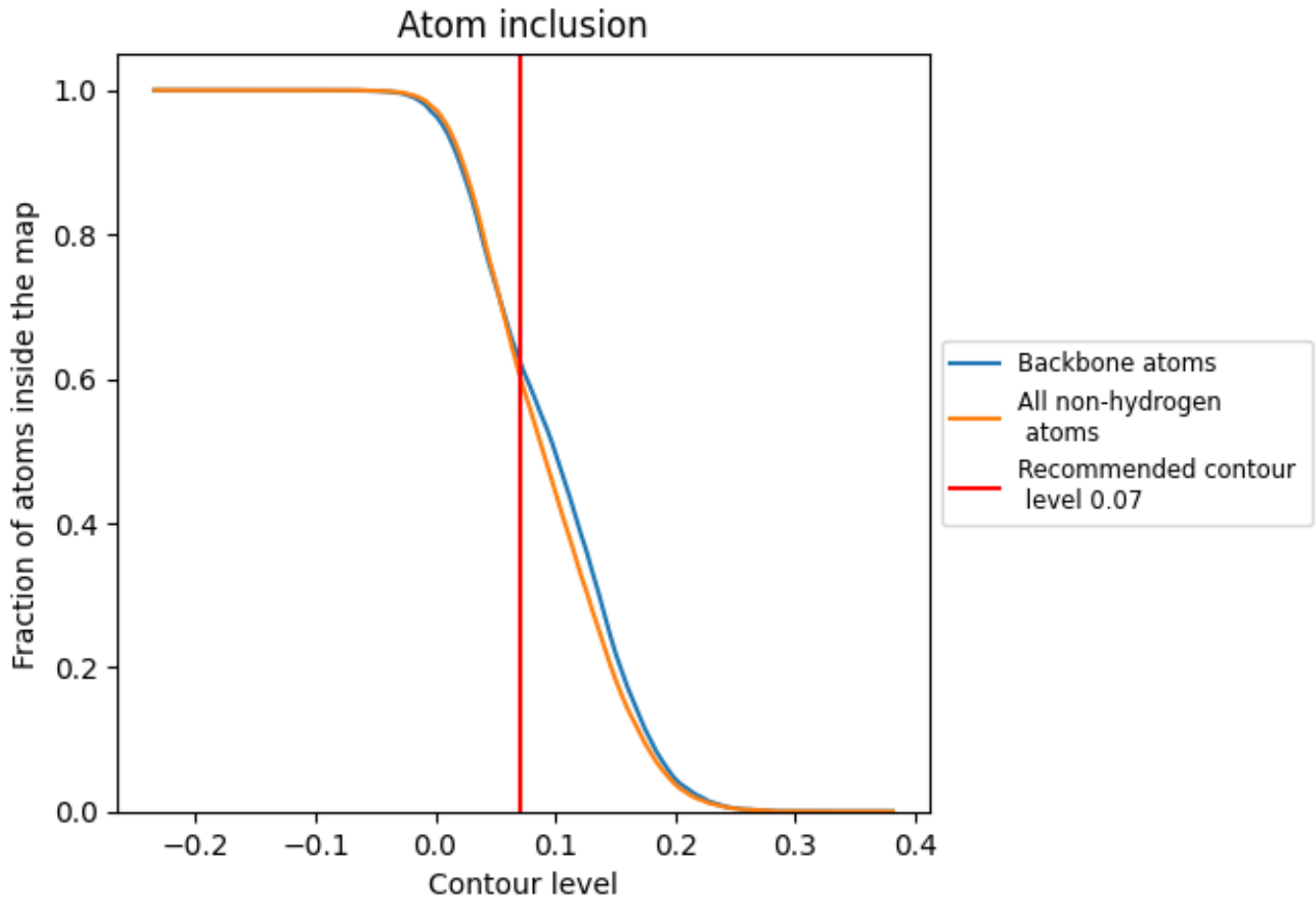
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.07).

9.4 Atom inclusion (i)



At the recommended contour level, 63% of all backbone atoms, 61% 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 (0.07) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6064	0.4920
A	0.5970	0.4860
B	0.5417	0.4770
C	0.7312	0.5380