wwPDB EM Validation Summary Report (i)

Aug 8, 2026 – 12:59 PM EDT

PDB ID	:	9YNK / pdb_00009ynk
EMDB ID	:	EMD-73210
Title	:	Human type 2 IP3 receptor in the inactive-like state (IP3/ATP/Ca2+)
Authors	:	Liu, C.; Lan, Y.; Tang, Q.; Karakas, E.
Deposited on	:	2025-10-10
Resolution	:	3.42 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:

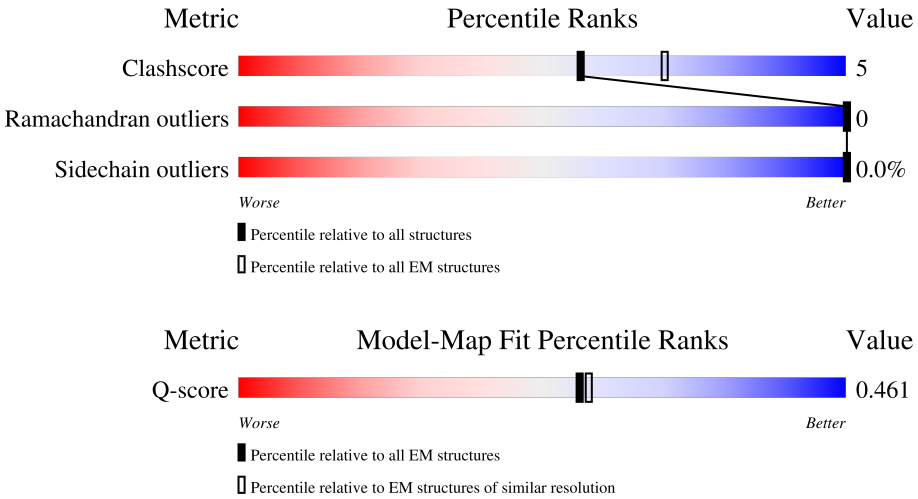
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

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 3.42 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	13959 (2.92 - 3.92)

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	2745	66% 10% 24%
1	B	2745	50% 7% 43%
1	C	2745	22% 74%
1	D	2745	13% 85%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 38038 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 Inositol 1,4,5-trisphosphate-gated calcium channel ITPR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2081	Total	C	N	O	S	0	0
			16280	10383	2814	2989	94		
1	B	1576	Total	C	N	O	S	0	0
			12410	7941	2134	2261	74		
1	C	712	Total	C	N	O	S	0	0
			5780	3728	974	1041	37		
1	D	416	Total	C	N	O	S	0	0
			3413	2239	561	594	19		

There are 176 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2702	ALA	-	expression tag	UNP Q14571
A	2703	SER	-	expression tag	UNP Q14571
A	2704	ALA	-	expression tag	UNP Q14571
A	2705	SER	-	expression tag	UNP Q14571
A	2706	ASN	-	expression tag	UNP Q14571
A	2707	GLY	-	expression tag	UNP Q14571
A	2708	LEU	-	expression tag	UNP Q14571
A	2709	VAL	-	expression tag	UNP Q14571
A	2710	PRO	-	expression tag	UNP Q14571
A	2711	ARG	-	expression tag	UNP Q14571
A	2712	GLY	-	expression tag	UNP Q14571
A	2713	SER	-	expression tag	UNP Q14571
A	2714	ALA	-	expression tag	UNP Q14571
A	2715	ALA	-	expression tag	UNP Q14571
A	2716	ALA	-	expression tag	UNP Q14571
A	2717	GLY	-	expression tag	UNP Q14571
A	2718	TRP	-	expression tag	UNP Q14571
A	2719	SER	-	expression tag	UNP Q14571
A	2720	HIS	-	expression tag	UNP Q14571
A	2721	PRO	-	expression tag	UNP Q14571
A	2722	GLN	-	expression tag	UNP Q14571
A	2723	PHE	-	expression tag	UNP Q14571

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	2724	GLU	-	expression tag	UNP Q14571
A	2725	LYS	-	expression tag	UNP Q14571
A	2726	GLY	-	expression tag	UNP Q14571
A	2727	GLY	-	expression tag	UNP Q14571
A	2728	GLY	-	expression tag	UNP Q14571
A	2729	SER	-	expression tag	UNP Q14571
A	2730	GLY	-	expression tag	UNP Q14571
A	2731	GLY	-	expression tag	UNP Q14571
A	2732	GLY	-	expression tag	UNP Q14571
A	2733	SER	-	expression tag	UNP Q14571
A	2734	GLY	-	expression tag	UNP Q14571
A	2735	GLY	-	expression tag	UNP Q14571
A	2736	SER	-	expression tag	UNP Q14571
A	2737	ALA	-	expression tag	UNP Q14571
A	2738	TRP	-	expression tag	UNP Q14571
A	2739	SER	-	expression tag	UNP Q14571
A	2740	HIS	-	expression tag	UNP Q14571
A	2741	PRO	-	expression tag	UNP Q14571
A	2742	GLN	-	expression tag	UNP Q14571
A	2743	PHE	-	expression tag	UNP Q14571
A	2744	GLU	-	expression tag	UNP Q14571
A	2745	LYS	-	expression tag	UNP Q14571
B	2702	ALA	-	expression tag	UNP Q14571
B	2703	SER	-	expression tag	UNP Q14571
B	2704	ALA	-	expression tag	UNP Q14571
B	2705	SER	-	expression tag	UNP Q14571
B	2706	ASN	-	expression tag	UNP Q14571
B	2707	GLY	-	expression tag	UNP Q14571
B	2708	LEU	-	expression tag	UNP Q14571
B	2709	VAL	-	expression tag	UNP Q14571
B	2710	PRO	-	expression tag	UNP Q14571
B	2711	ARG	-	expression tag	UNP Q14571
B	2712	GLY	-	expression tag	UNP Q14571
B	2713	SER	-	expression tag	UNP Q14571
B	2714	ALA	-	expression tag	UNP Q14571
B	2715	ALA	-	expression tag	UNP Q14571
B	2716	ALA	-	expression tag	UNP Q14571
B	2717	GLY	-	expression tag	UNP Q14571
B	2718	TRP	-	expression tag	UNP Q14571
B	2719	SER	-	expression tag	UNP Q14571
B	2720	HIS	-	expression tag	UNP Q14571
B	2721	PRO	-	expression tag	UNP Q14571

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	2722	GLN	-	expression tag	UNP Q14571
B	2723	PHE	-	expression tag	UNP Q14571
B	2724	GLU	-	expression tag	UNP Q14571
B	2725	LYS	-	expression tag	UNP Q14571
B	2726	GLY	-	expression tag	UNP Q14571
B	2727	GLY	-	expression tag	UNP Q14571
B	2728	GLY	-	expression tag	UNP Q14571
B	2729	SER	-	expression tag	UNP Q14571
B	2730	GLY	-	expression tag	UNP Q14571
B	2731	GLY	-	expression tag	UNP Q14571
B	2732	GLY	-	expression tag	UNP Q14571
B	2733	SER	-	expression tag	UNP Q14571
B	2734	GLY	-	expression tag	UNP Q14571
B	2735	GLY	-	expression tag	UNP Q14571
B	2736	SER	-	expression tag	UNP Q14571
B	2737	ALA	-	expression tag	UNP Q14571
B	2738	TRP	-	expression tag	UNP Q14571
B	2739	SER	-	expression tag	UNP Q14571
B	2740	HIS	-	expression tag	UNP Q14571
B	2741	PRO	-	expression tag	UNP Q14571
B	2742	GLN	-	expression tag	UNP Q14571
B	2743	PHE	-	expression tag	UNP Q14571
B	2744	GLU	-	expression tag	UNP Q14571
B	2745	LYS	-	expression tag	UNP Q14571
C	2702	ALA	-	expression tag	UNP Q14571
C	2703	SER	-	expression tag	UNP Q14571
C	2704	ALA	-	expression tag	UNP Q14571
C	2705	SER	-	expression tag	UNP Q14571
C	2706	ASN	-	expression tag	UNP Q14571
C	2707	GLY	-	expression tag	UNP Q14571
C	2708	LEU	-	expression tag	UNP Q14571
C	2709	VAL	-	expression tag	UNP Q14571
C	2710	PRO	-	expression tag	UNP Q14571
C	2711	ARG	-	expression tag	UNP Q14571
C	2712	GLY	-	expression tag	UNP Q14571
C	2713	SER	-	expression tag	UNP Q14571
C	2714	ALA	-	expression tag	UNP Q14571
C	2715	ALA	-	expression tag	UNP Q14571
C	2716	ALA	-	expression tag	UNP Q14571
C	2717	GLY	-	expression tag	UNP Q14571
C	2718	TRP	-	expression tag	UNP Q14571
C	2719	SER	-	expression tag	UNP Q14571

Continued on next page...

Continued from previous page...

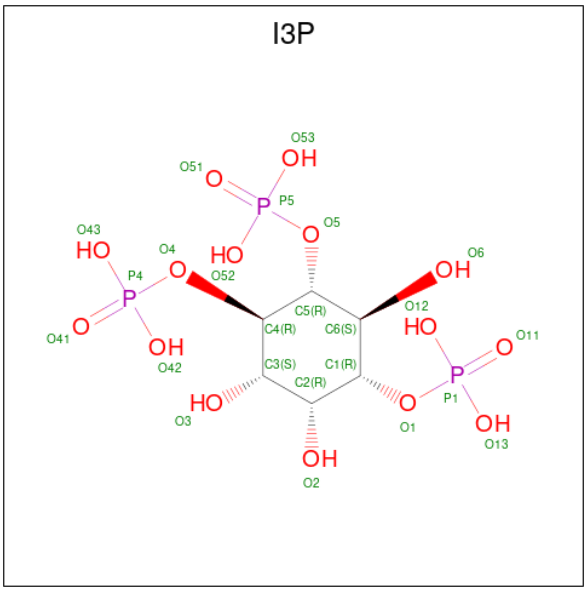
Chain	Residue	Modelled	Actual	Comment	Reference
C	2720	HIS	-	expression tag	UNP Q14571
C	2721	PRO	-	expression tag	UNP Q14571
C	2722	GLN	-	expression tag	UNP Q14571
C	2723	PHE	-	expression tag	UNP Q14571
C	2724	GLU	-	expression tag	UNP Q14571
C	2725	LYS	-	expression tag	UNP Q14571
C	2726	GLY	-	expression tag	UNP Q14571
C	2727	GLY	-	expression tag	UNP Q14571
C	2728	GLY	-	expression tag	UNP Q14571
C	2729	SER	-	expression tag	UNP Q14571
C	2730	GLY	-	expression tag	UNP Q14571
C	2731	GLY	-	expression tag	UNP Q14571
C	2732	GLY	-	expression tag	UNP Q14571
C	2733	SER	-	expression tag	UNP Q14571
C	2734	GLY	-	expression tag	UNP Q14571
C	2735	GLY	-	expression tag	UNP Q14571
C	2736	SER	-	expression tag	UNP Q14571
C	2737	ALA	-	expression tag	UNP Q14571
C	2738	TRP	-	expression tag	UNP Q14571
C	2739	SER	-	expression tag	UNP Q14571
C	2740	HIS	-	expression tag	UNP Q14571
C	2741	PRO	-	expression tag	UNP Q14571
C	2742	GLN	-	expression tag	UNP Q14571
C	2743	PHE	-	expression tag	UNP Q14571
C	2744	GLU	-	expression tag	UNP Q14571
C	2745	LYS	-	expression tag	UNP Q14571
D	2702	ALA	-	expression tag	UNP Q14571
D	2703	SER	-	expression tag	UNP Q14571
D	2704	ALA	-	expression tag	UNP Q14571
D	2705	SER	-	expression tag	UNP Q14571
D	2706	ASN	-	expression tag	UNP Q14571
D	2707	GLY	-	expression tag	UNP Q14571
D	2708	LEU	-	expression tag	UNP Q14571
D	2709	VAL	-	expression tag	UNP Q14571
D	2710	PRO	-	expression tag	UNP Q14571
D	2711	ARG	-	expression tag	UNP Q14571
D	2712	GLY	-	expression tag	UNP Q14571
D	2713	SER	-	expression tag	UNP Q14571
D	2714	ALA	-	expression tag	UNP Q14571
D	2715	ALA	-	expression tag	UNP Q14571
D	2716	ALA	-	expression tag	UNP Q14571
D	2717	GLY	-	expression tag	UNP Q14571

Continued on next page...

Continued from previous page...

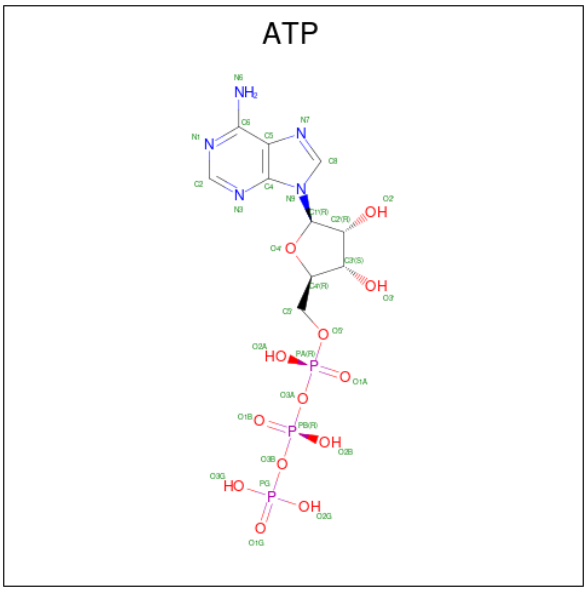
Chain	Residue	Modelled	Actual	Comment	Reference
D	2718	TRP	-	expression tag	UNP Q14571
D	2719	SER	-	expression tag	UNP Q14571
D	2720	HIS	-	expression tag	UNP Q14571
D	2721	PRO	-	expression tag	UNP Q14571
D	2722	GLN	-	expression tag	UNP Q14571
D	2723	PHE	-	expression tag	UNP Q14571
D	2724	GLU	-	expression tag	UNP Q14571
D	2725	LYS	-	expression tag	UNP Q14571
D	2726	GLY	-	expression tag	UNP Q14571
D	2727	GLY	-	expression tag	UNP Q14571
D	2728	GLY	-	expression tag	UNP Q14571
D	2729	SER	-	expression tag	UNP Q14571
D	2730	GLY	-	expression tag	UNP Q14571
D	2731	GLY	-	expression tag	UNP Q14571
D	2732	GLY	-	expression tag	UNP Q14571
D	2733	SER	-	expression tag	UNP Q14571
D	2734	GLY	-	expression tag	UNP Q14571
D	2735	GLY	-	expression tag	UNP Q14571
D	2736	SER	-	expression tag	UNP Q14571
D	2737	ALA	-	expression tag	UNP Q14571
D	2738	TRP	-	expression tag	UNP Q14571
D	2739	SER	-	expression tag	UNP Q14571
D	2740	HIS	-	expression tag	UNP Q14571
D	2741	PRO	-	expression tag	UNP Q14571
D	2742	GLN	-	expression tag	UNP Q14571
D	2743	PHE	-	expression tag	UNP Q14571
D	2744	GLU	-	expression tag	UNP Q14571
D	2745	LYS	-	expression tag	UNP Q14571

- Molecule 2 is D-MYO-INOSITOL-1,4,5-TRIPHOSPHATE (CCD ID: I3P) (formula: $C_6H_{15}O_{15}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	O	P	0
			24	6	15	3	

- Molecule 3 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$) (labeled as "Ligand of Interest" by depositor).



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

Continued on next page...

Continued from previous page...

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

- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	1	Total	Zn	0
			1	1	
4	B	1	Total	Zn	0
			1	1	
4	C	1	Total	Zn	0
			1	1	
4	D	1	Total	Zn	0
			1	1	

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Ca	0
			1	1	
5	B	1	Total	Ca	0
			1	1	
5	C	1	Total	Ca	0
			1	1	

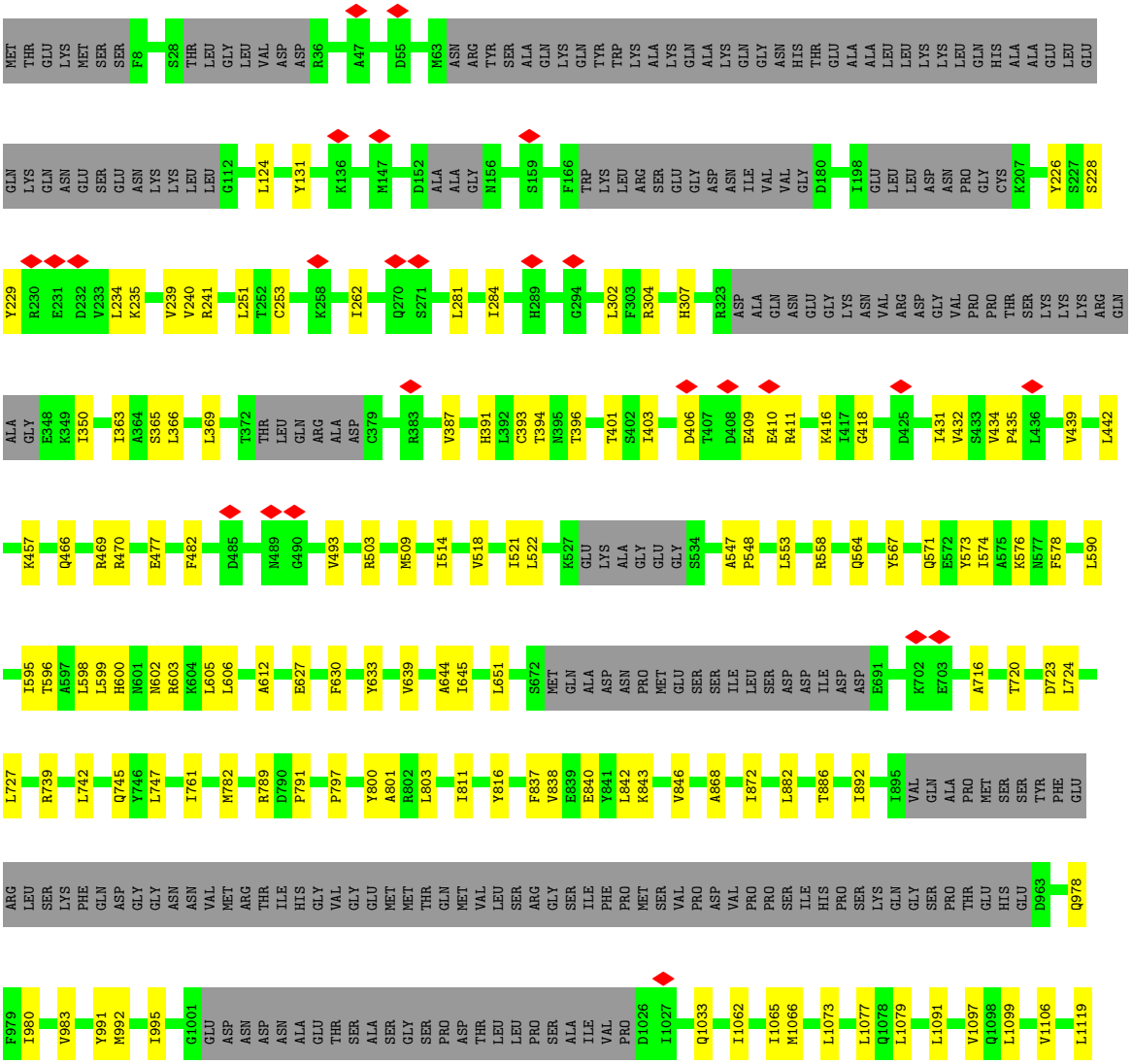
3 Residue-property plots (i)

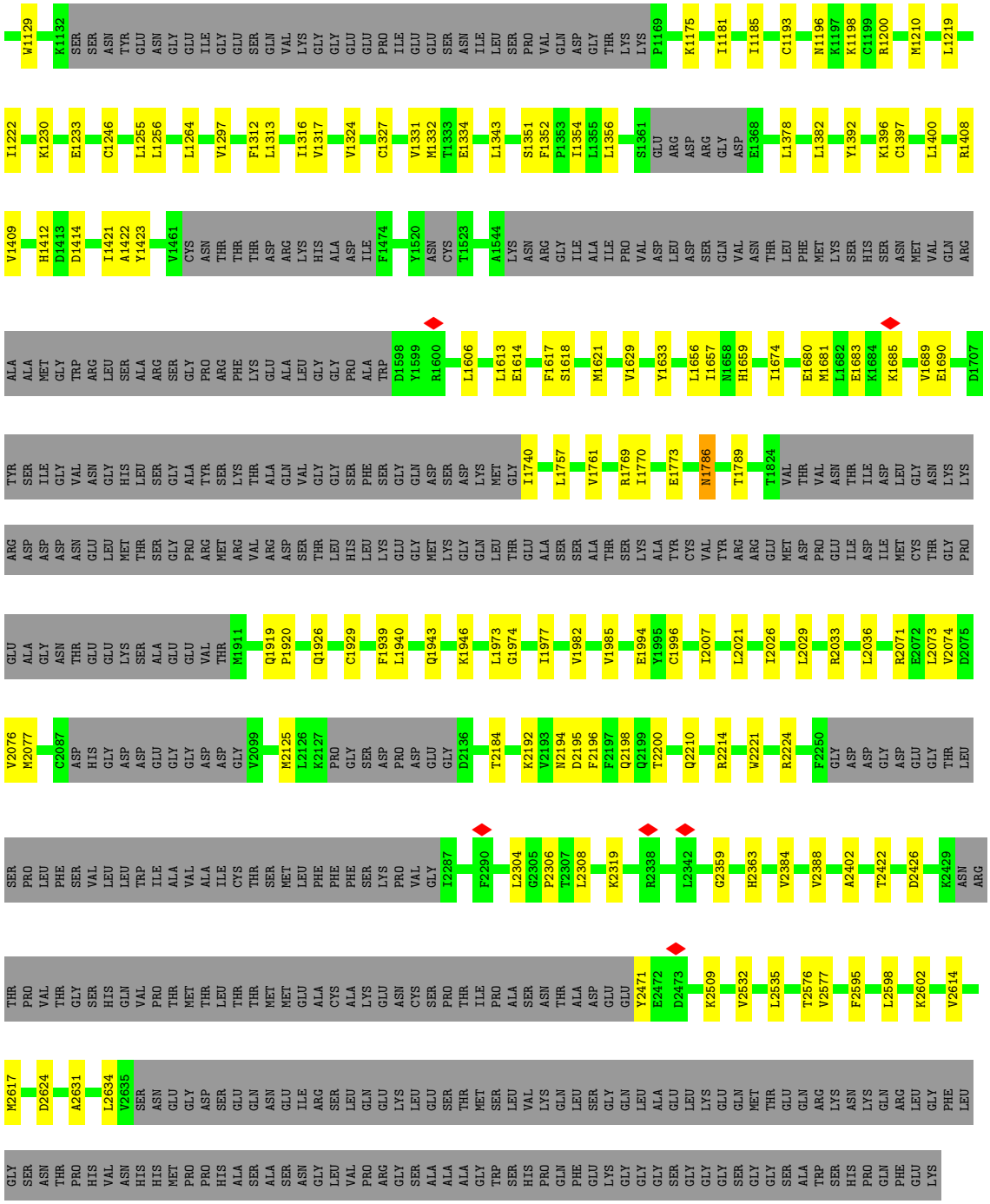
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Inositol 1,4,5-trisphosphate-gated calcium channel ITPR2

Chain A:

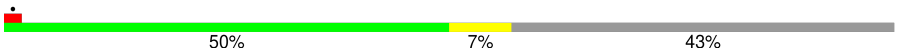


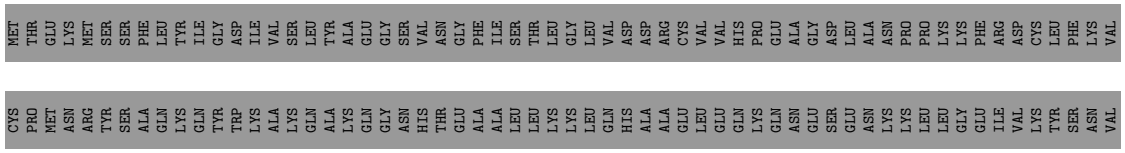


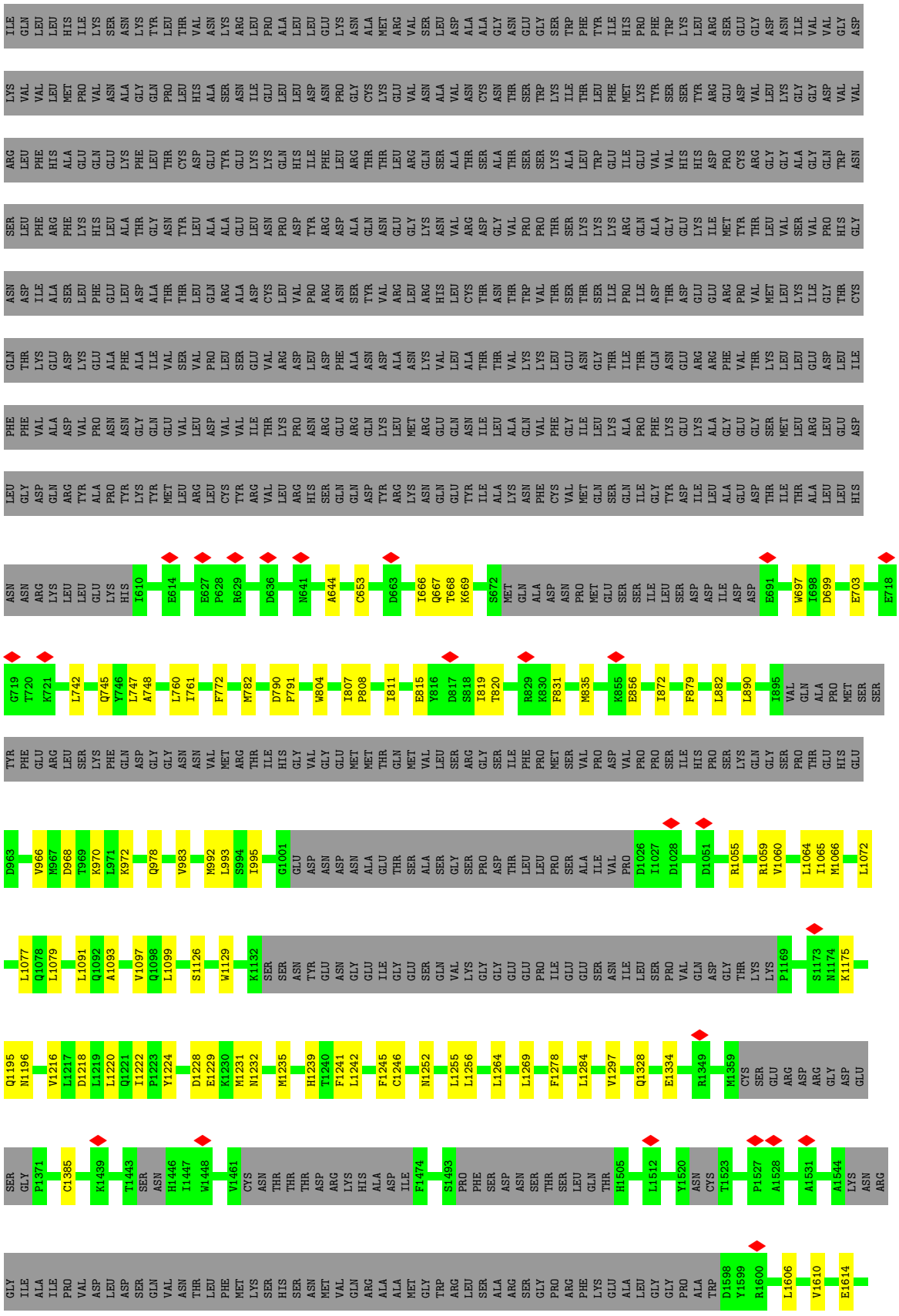


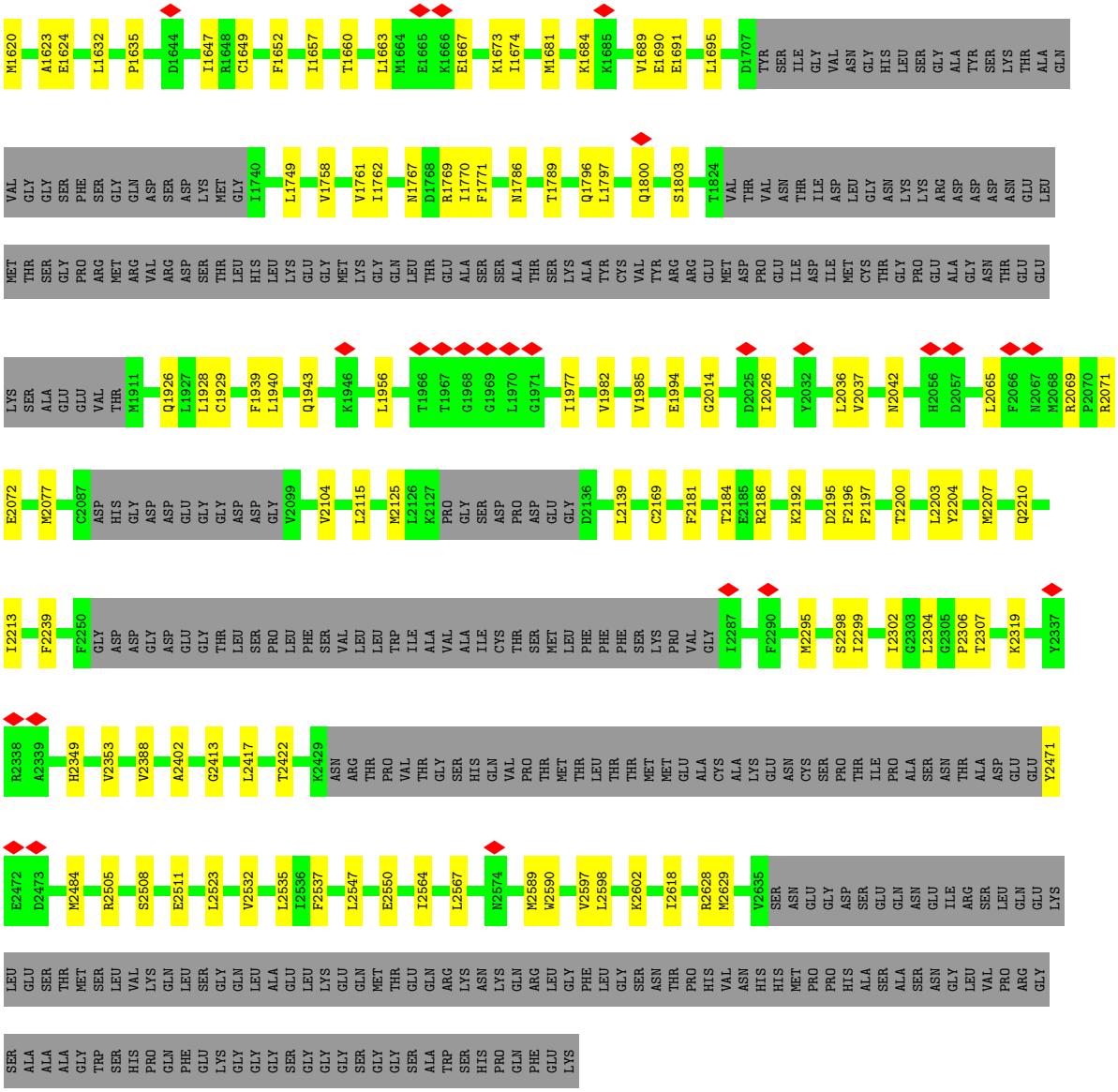
• Molecule 1: Inositol 1,4,5-trisphosphate-gated calcium channel ITPR2

Chain B:





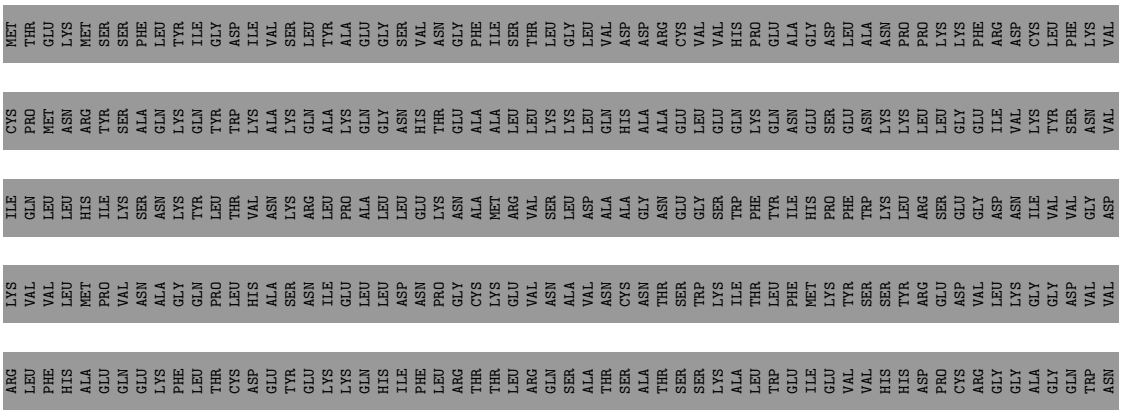


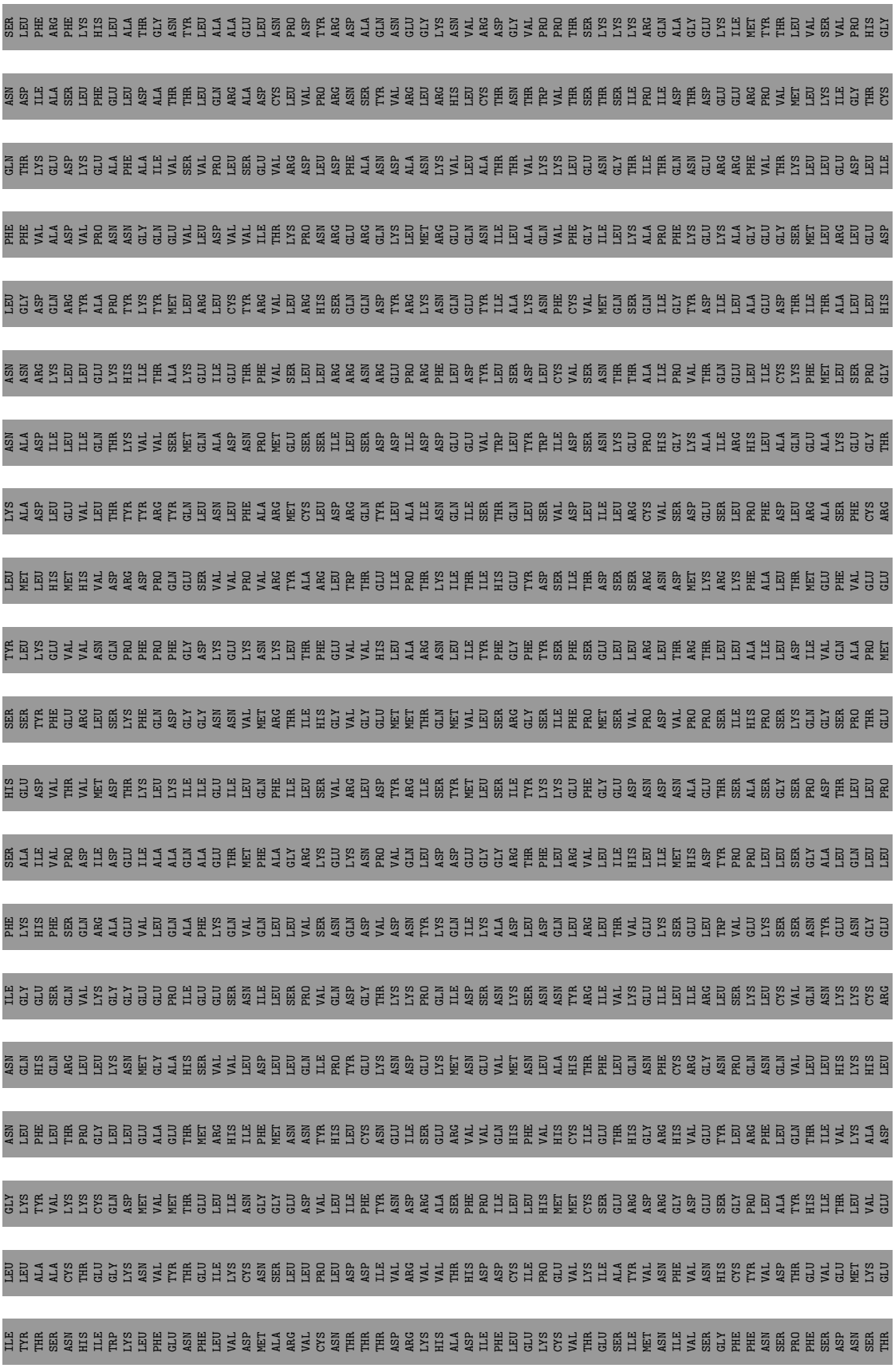


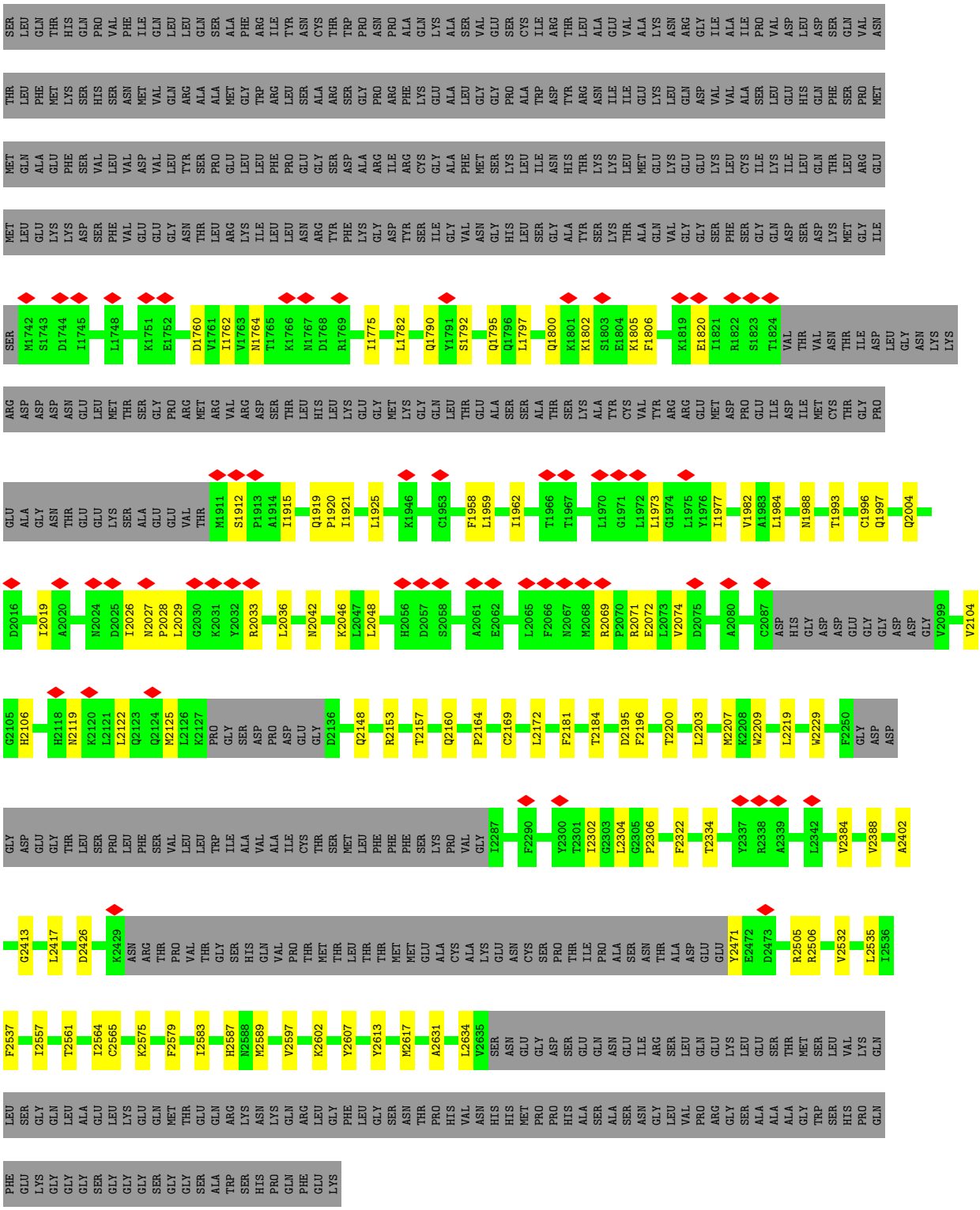
• Molecule 1: Inositol 1,4,5-trisphosphate-gated calcium channel ITPR2

Chain C:







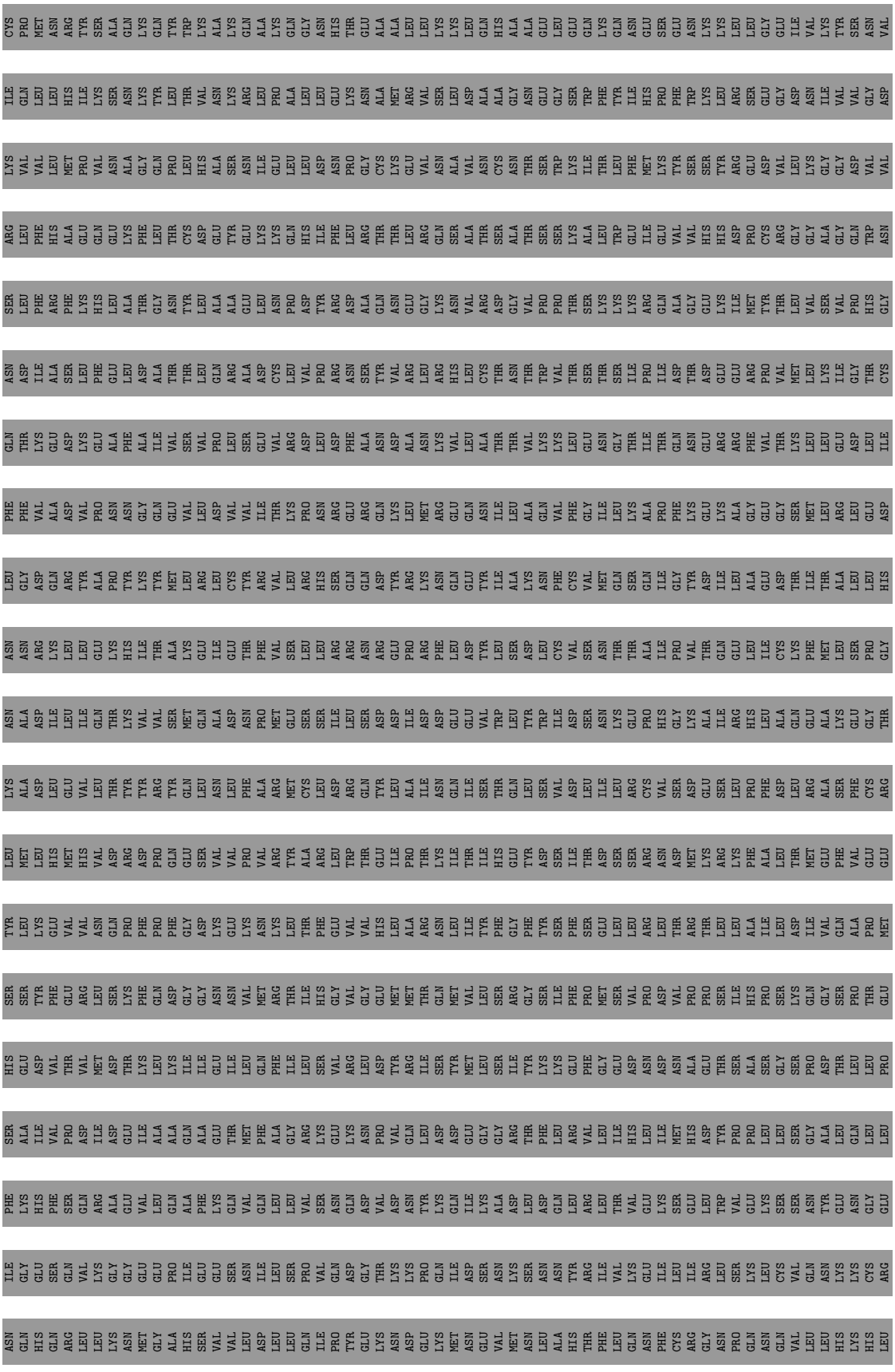


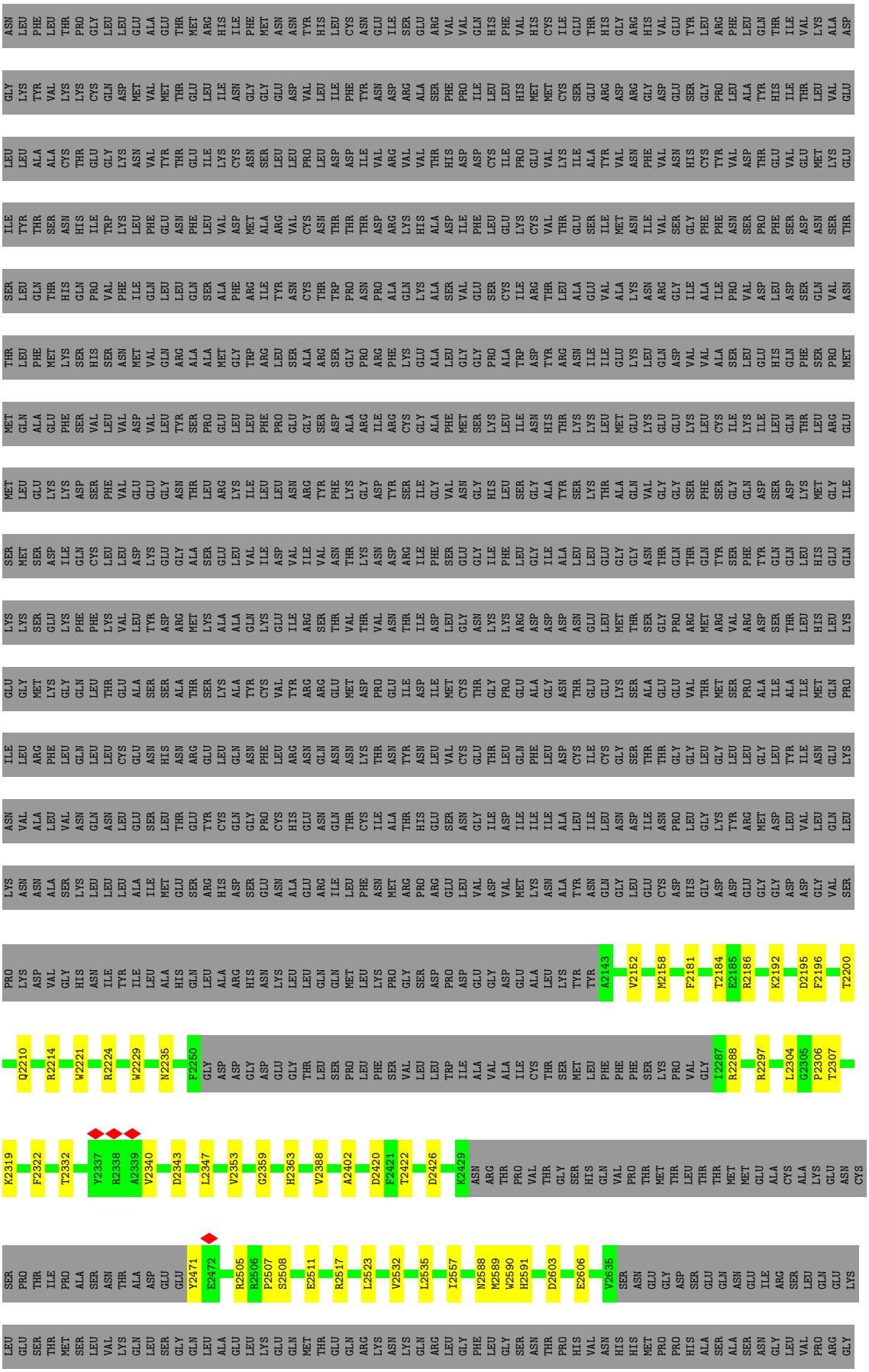
• Molecule 1: Inositol 1,4,5-trisphosphate-gated calcium channel ITPR2

Chain D:






CYS PRO MET ASN ARG TYR SER ALA GLN LYS GLN TYR TRP LYS ALA LYS GLN ALA LYS GLN GLY ASN HIS THR GLU ALA ALA LEU LEU LYS LYS LEU GLN HIS ALA GLY GLU LEU GLU GLN LYS GLN ASN GLU SER GLU ASN LYS LYS LEU LEU GLY GLU ILE VAL LYS TYR SER ASN VAL
ILE GLN LEU LEU HIS ILE LYS SER ASN LYS TYR LEU THR VAL ASN LYS ARG LEU PRO ALA LEU LEU GLU ASN HIS ALA ASN PRO GLY CYS LYS GLU VAL ASN ALA VAL ASN CYS ASN THR SER TRP LYS ILE THR LEU PHE MET LYS TYR SER SER TYR ARG GLU ASP PRO CYS ARG GLY GLY ASN ILE VAL VAL GLY ASP
LYS VAL VAL LEU MET PRO VAL ASN ALA GLY GLN PRO LEU HIS ALA SER ASN ILE GLU LEU LEU ASP ASN PRO GLY CYS LYS GLU VAL ASN ALA VAL ASN ASN CYS ASN THR SER TRP LYS ILE THR LEU PHE MET LYS TYR SER SER TYR ARG GLU ASP PRO GLY GLN LEU LYS GLY GLY VAL VAL
ARG LEU PHE HIS ALA GLU GLN GLU LYS PHE LEU THR CYS ASP GLU TYR GLU LYS LYS GLN HIS ILE PHE LEU ARG THR THR LEU ARG GLN SER ALA THR SER SER LYS ALA LEU TRP GLU ILE GLU VAL HIS HIS ASP PRO CYS ARG GLY GLY GLN TRP ASN
SER LEU PHE HIS LEU ALA THR GLY ASN TYR LEU ALA ALA GLU GLY LYS ASN VAL ARG ASP SER LYS LYS LYS ASN VAL ARG ASP ASP GLY VAL PRO PRO SER THR SER LYS LYS ARG GLN ALA ALA GLY GLU HIS VAL GLU LYS ILE MET TYR THR LEU VAL SER VAL PRO HIS GLY
ASN ASP ILE ALA SER LEU PHE GLU LEU ALA THR THR LEU GLN ARG ALA ASP CYS LEU VAL PRO ARG ASN SER TYR VAL ARG LEU LEU ARG ASN SER THR ASN THR TRP VAL THR SER THR SER THR ASP GLU GLU ARG PHE VAL THR LYS LEU LEU GLU ASP LEU ILE THR GLY
GLN THR LYS GLU ASP LYS GLU ALA PHE ALA ILE VAL SER VAL PRO LEU SER GLU VAL ARG ASP LEU ASP PHE ALA ASN ARG GLU ARG GLN LYS LEU MET ARG GLU GLN ASN ILE THR VAL LYS LYS LEU GLU ASN GLY THR ILE THR GLN ASN GLU ARG ARG PHE VAL THR LYS LEU LEU GLU ASP LEU GLU
PHE PHE VAL ALA ASP VAL PRO ASN ASN GLY GLN GLU VAL LEU ASP VAL PRO ASN ARG GLN LYS LEU MET ARG GLU GLN ASN ILE LEU ALA GLN VAL PHE GLY ILE LEU LYS ALA PRO PHE LYS GLU ALA GLY GLU GLY SER MET LEU LEU GLU GLU ASP
LEU GLY ASP GLN ARG TYR ALA PRO TYR LYS TYR MET LEU ARG LEU CYS TYR ARG VAL LEU ARG HIS SER GLN GLN ASP TYR ARG LYS ASN GLN GLU TYR ILE ALA LYS ASN PHE CYS VAL MET GLN SER GLN ILE GLY TYR ASP ILE LEU GLY SER MET LEU ARG LEU LEU HIS
ASN ASN ARG LYS LEU LEU GLU LYS HIS ILE THR ALA LYS GLU ILE GLU THR PHE VAL SER LEU LEU ARG ARG ASN ARG GLU PRO ARG PHE LEU ASP TYR LEU SER ASP LEU CYS VAL SER ASN THR THR ALA ILE PRO VAL THR GLN GLU LEU ILE CYS LYS PHE MET LEU SER PRO GLY
ASN ALA ASP ILE LEU LEU ILE GLN THR LYS VAL VAL SER MET GLN ALA ASP ASN PRO MET GLU SER SER ILE LEU SER ASP ILE ASP ASP GLU GLU VAL TRP LEU TYR TRP ILE ASP SER ASN LYS GLU PRO HIS GLY LYS ALA ILE ARG HIS LEU ALA GLN GLU ALA LYS GLU GLY THR
LYS ALA ASP LEU GLU VAL TYR TYR ARG TYR GLN LEU ASN LEU PHE ALA ARG MET CYS LEU ASP ARG GLN TYR LEU ALA ILE ASN GLN LEU SER VAL ASP LEU ILE LEU ARG CYS VAL SER ASP ILE PHE ASP ASP ARG ASP ILE ILE ASP ASP GLU GLU GLN ILE ASN LEU ARG ILE SER THR GLU LEU ILE ASP ASP GLU GLU VAL TRP LEU TYR TRP ILE ASP SER ASN LYS GLU PRO HIS GLY LYS ALA ILE ARG HIS LEU ALA GLN GLU ALA LYS GLU GLY THR
LEU MET LEU HIS MET HIS VAL ASP ARG ASP PRO PRO GLN GLU GLN LEU TRP THR GLU ILE PRO THR LYS ILE THR ILE HIS GLU TYR ASP SER SER ARG ASN ASP MET LYS ARG LYS PHE PHE ASP PHE SER PHE SER ASP GLU LEU LEU ARG THR ASP MET LYS ARG LEU PRO PHE ASP ASP LEU THR MET GLU PHE VAL GLU GLU
TYR LEU LYS GLU VAL VAL ASN GLN PRO PHE PRO PHE GLY ASP LYS GLU VAL ASN LYS LEU THR PHE SER ALA ARG ASN LEU ILE THR PHE GLY PHE TYR SER PHE SER GLU LEU LEU ARG LEU THR ARG THR LEU LEU ALA ILE LEU LEU ASP ILE VAL GLN ALA PRO MET
SER SER TYR PHE GLU ARG LEU SER LYS PHE GLN ASP GLY GLY ASN ASN VAL ASN GLY VAL HIS LEU GLU MET MET THR GLN MET VAL LEU SER ARG GLY PHE SER ILE PHE PRO MET SER VAL PRO ASP VAL PRO PRO SER ILE HIS PRO SER LYS GLN GLY SER PRO PRO THR GLU
HIS GLU ASP VAL THR LYS LEU LYS ILE ILE GLU LEU GLN PHE ILE LEU SER VAL ARG LEU ASP TYR ARG ILE SER TYR MET LEU SER ILE LYS LYS GLU PHE GLY GLU ASP ASN ASP ASN ALA GLU THR SER ALA SER GLY SER PRO ASP THR LEU LEU PRO
SER ALA ILE VAL PRO ASP ILE ASP GLU LYS ASN PRO VAL GLN LEU ASP ASP GLU GLY GLY ARG THR PHE LEU ARG VAL LEU ILE HIS LEU GLU ILE MET HIS ASP TYR PRO PRO LEU LEU SER GLY ALA LEU GLN LEU LEU
PHE LYS HIS PHE SER GLN ARG ALA GLU VAL LEU GLN GLN ALA PHE LYS GLN VAL GLN LEU LEU VAL SER ASN GLN ASP VAL ASP ASN TYR LYS GLN ILE LYS ALA ASP LEU ASP GLN LEU ARG LEU THR VAL GLU LYS SER GLU LEU TRP VAL GLU LYS SER SER ASN TYR GLU ASN GLY GLU
ILE GLY GLU SER GLN VAL LYS GLY GLY GLU GLU PRO ILE GLU GLU SER ASN ILE LEU SER PRO VAL GLN ASP GLY THR LYS LYS PRO GLN ILE ASP SER ASN ASP ILE ASN ASP ILE ASN TYR ARG ILE VAL LYS GLU ILE LEU ARG ILE CYS LEU LYS LYS CYS ARG
ASN GLN HIS GLN ARG LEU LEU LYS ASN MET GLY ALA HIS SER VAL VAL LEU ASP LEU LEU GLN PRO TYR GLU LYS ASN ASP GLU LYS MET ASN GLU VAL MET ASN LEU ALA HIS THR PHE LEU GLN ASN PHE CYS ARG GLY ASN PRO GLN LYS LEU LEU HIS LYS LEU


A2143
V2152
M2158
F2181
T2184
E2185
R2186
K2192
D2195
F2196
T2200
Q2210
R2214
W2221
R2224
W2229
N2235
P2250
I2287
R2288
R2297
L2304
G2305
P2306
T2307
K2319
F2322
T2332
Y2337
R2338
A2339
V2340
D2343
L2347
V2353
G2359
H2363
V2388
A2402
D2420
F2421
T2422
D2426
K2429
Y2471
E2472
R2505
R2506
P2507
S2508
E2511
R2517
L2523
V2532
L2535
I2557
N2588
M2589
W2590
H2591
D2603
E2606
V2635

SER
ALA
ALA
ALA
GLY
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS
GLY
GLY
GLY
SER
GLY
GLY
GLY
SER
GLY
GLY
SER
ALA
TRP
SER
HIS
PRO
GLN
PHE
GLU
LYS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	157230	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	54.7	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.808	Depositor
Minimum map value	-0.008	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.05	Depositor
Map size (Å)	420.864, 420.864, 420.864	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.822, 0.822, 0.822	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: I3P, ATP, ZN, CA

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	0.15	0/16553	0.26	0/22384
1	B	0.14	0/12619	0.26	0/17050
1	C	0.14	0/5888	0.24	0/7952
1	D	0.15	0/3490	0.24	0/4723
All	All	0.14	0/38550	0.26	0/52109

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	16280	0	15838	161	0
1	B	12410	0	12160	121	0
1	C	5780	0	5850	65	0
1	D	3413	0	3464	37	0
2	A	24	0	9	0	0
3	A	31	0	12	0	0
3	B	31	0	12	0	0
3	C	31	0	12	1	0
3	D	31	0	12	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
All	All	38038	0	37369	367	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 5.

The worst 5 of 367 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:C:1962:ILE:HD13	1:C:1984:LEU:HD22	1.70	0.73
1:B:2628:ARG:HD2	1:B:2629:MET:HG2	1.71	0.73
1:D:2186:ARG:HG2	1:D:2192:LYS:HG2	1.71	0.72
1:B:2402:ALA:HB2	1:B:2532:VAL:HG11	1.73	0.71
1:A:2402:ALA:HB2	1:A:2532:VAL:HG11	1.73	0.70

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	2035/2745 (74%)	1964 (96%)	71 (4%)	0	100	100
1	B	1542/2745 (56%)	1487 (96%)	55 (4%)	0	100	100
1	C	700/2745 (26%)	678 (97%)	22 (3%)	0	100	100
1	D	410/2745 (15%)	398 (97%)	12 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4687/10980 (43%)	4527 (97%)	160 (3%)	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	1703/2448 (70%)	1702 (100%)	1 (0%)	88 88
1	B	1308/2448 (53%)	1308 (100%)	0	100 100
1	C	643/2448 (26%)	643 (100%)	0	100 100
1	D	378/2448 (15%)	378 (100%)	0	100 100
All	All	4032/9792 (41%)	4031 (100%)	1 (0%)	100 100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1786	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 38 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1997	GLN
1	D	2189	GLN
1	C	2067	ASN
1	C	2318	ASN
1	D	2496	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 oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 7 are monoatomic - leaving 5 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	ATP	C	2801	-	32,33,33	0.30	0	48,52,52	0.33	0
3	ATP	D	2801	-	32,33,33	0.33	0	48,52,52	0.33	0
3	ATP	B	2801	-	32,33,33	0.31	0	48,52,52	0.36	0
2	I3P	A	2801	-	24,24,24	2.16	3 (12%)	39,39,39	0.86	0
3	ATP	A	2802	-	32,33,33	0.31	0	48,52,52	0.32	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
3	ATP	C	2801	-	-	8/22/38/38	0/3/3/3
3	ATP	D	2801	-	-	5/22/38/38	0/3/3/3
3	ATP	B	2801	-	-	1/22/38/38	0/3/3/3
2	I3P	A	2801	-	-	2/15/39/39	0/1/1/1
3	ATP	A	2802	-	-	5/22/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2801	I3P	P4-O4	5.95	1.70	1.59
2	A	2801	I3P	P5-O5	5.85	1.69	1.59
2	A	2801	I3P	P1-O1	5.62	1.69	1.59

There are no bond angle outliers.

There are no chirality outliers.

5 of 21 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	2802	ATP	PB-O3B-PG-O2G
3	D	2801	ATP	PB-O3B-PG-O2G
3	C	2801	ATP	O4'-C4'-C5'-O5'
3	C	2801	ATP	C3'-C4'-C5'-O5'
3	A	2802	ATP	PB-O3A-PA-O1A

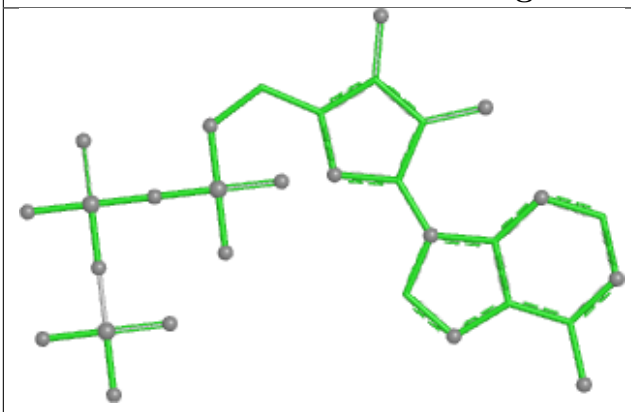
There are no ring outliers.

1 monomer is involved in 1 short contact:

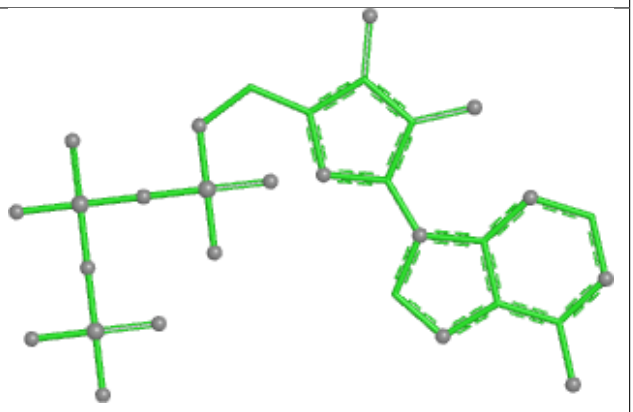
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2801	ATP	1	0

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.

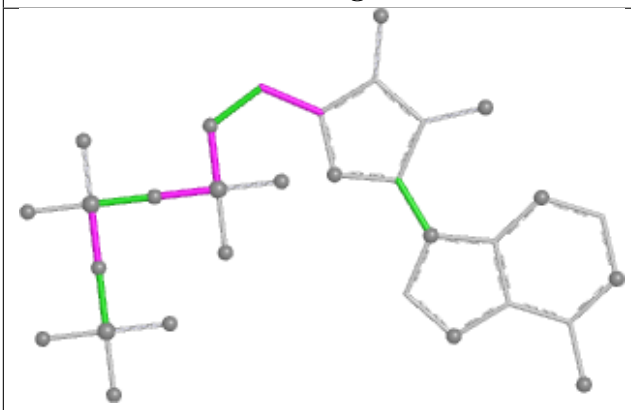
Ligand ATP C 2801



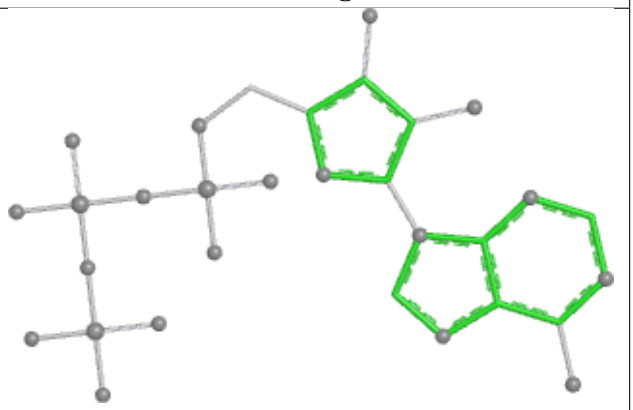
Bond lengths



Bond angles

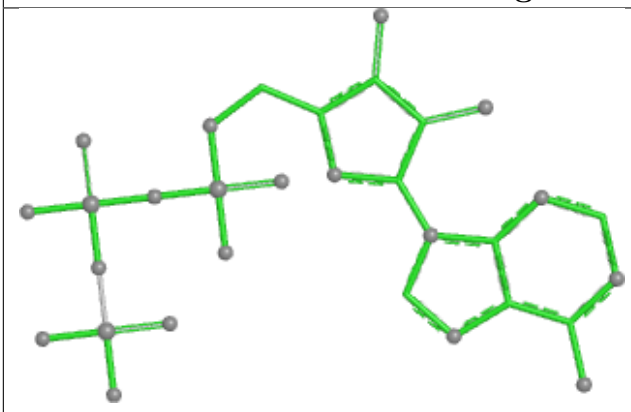


Torsions

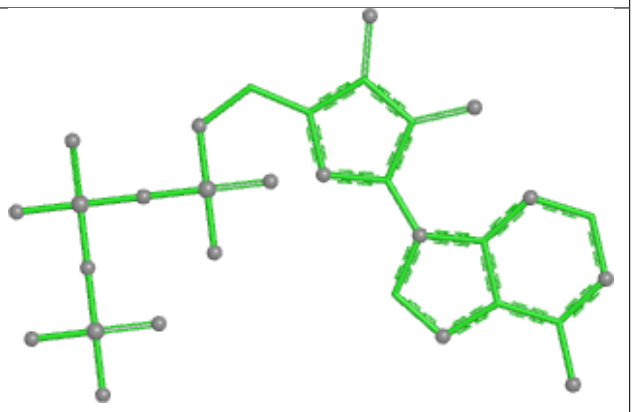


Rings

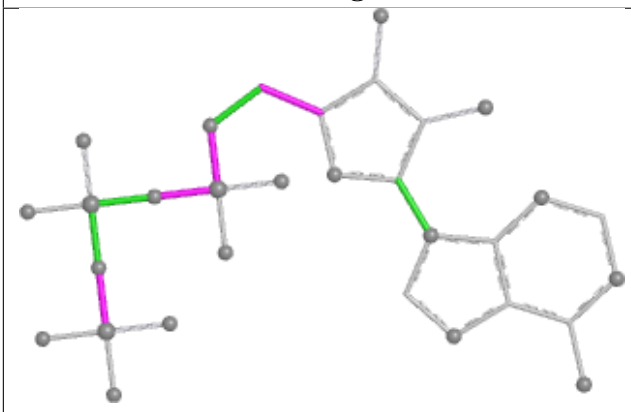
Ligand ATP D 2801



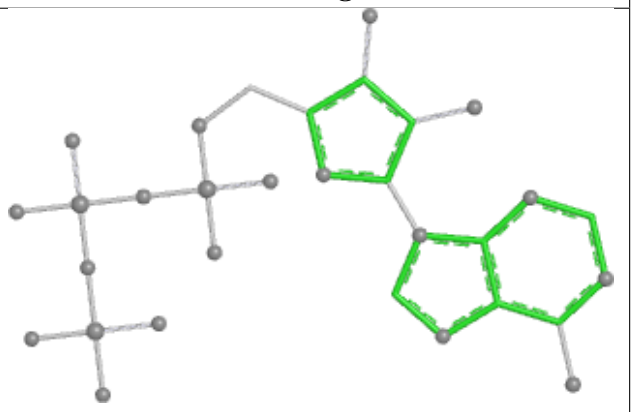
Bond lengths



Bond angles

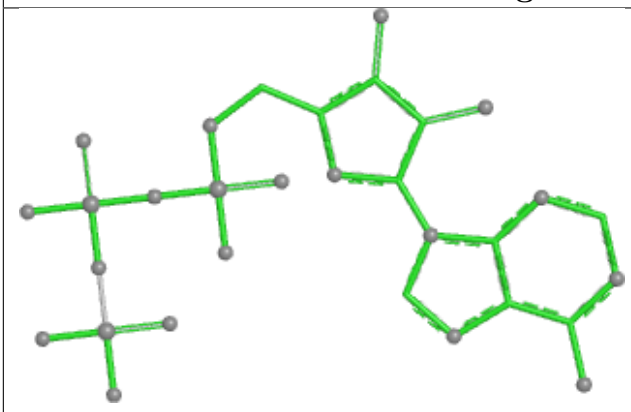


Torsions

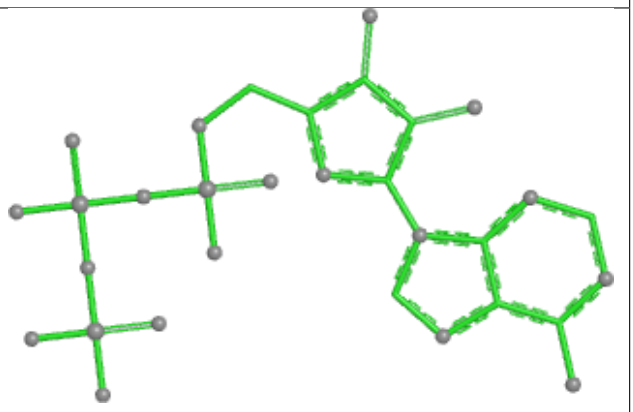


Rings

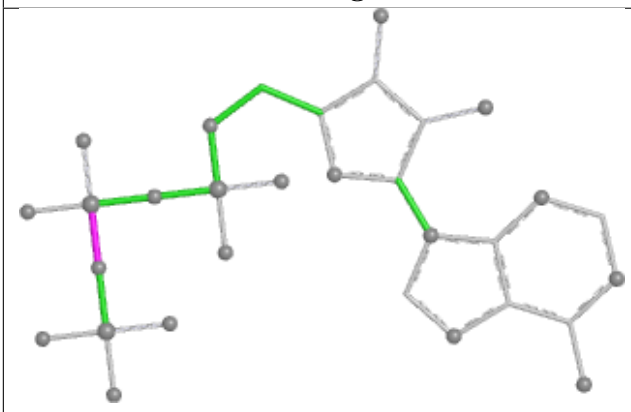
Ligand ATP B 2801



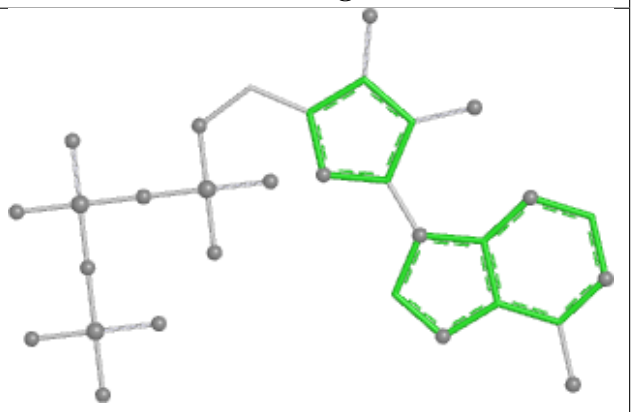
Bond lengths



Bond angles

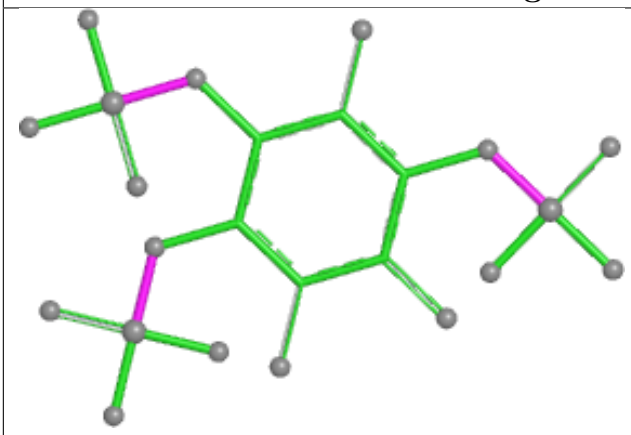


Torsions

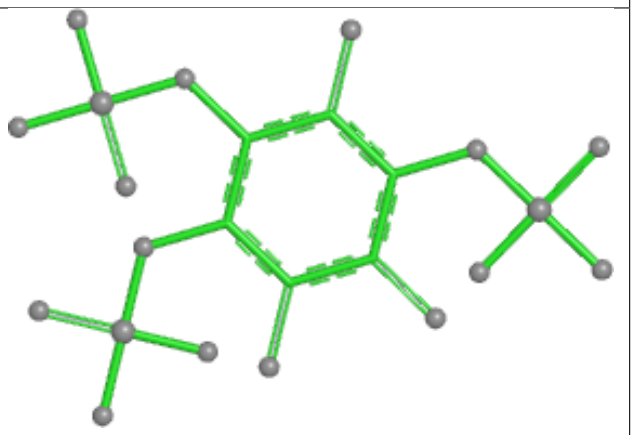


Rings

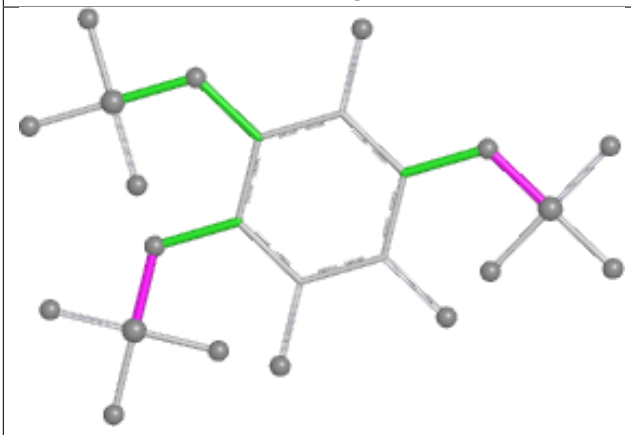
Ligand I3P A 2801



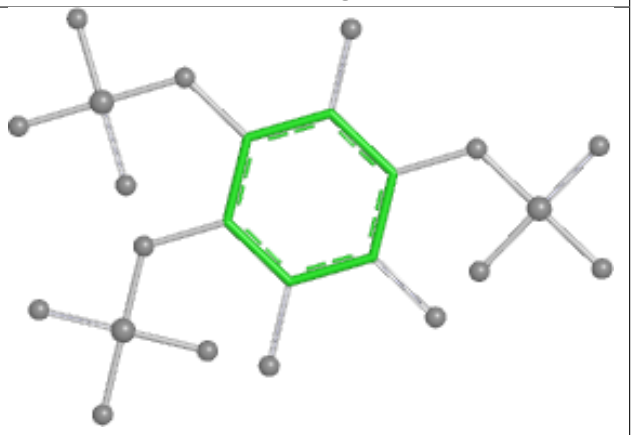
Bond lengths



Bond angles

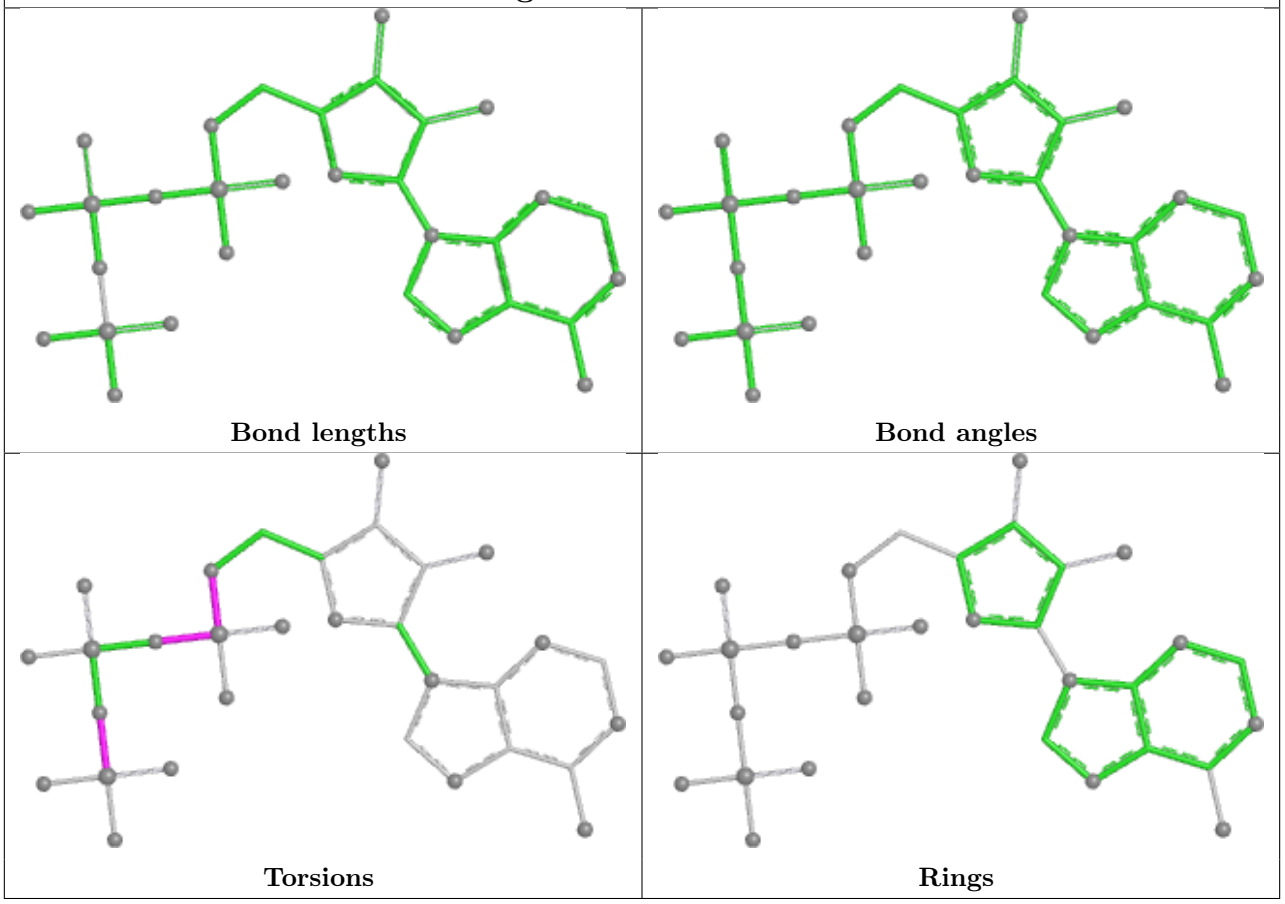


Torsions



Rings

Ligand ATP A 2802



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.

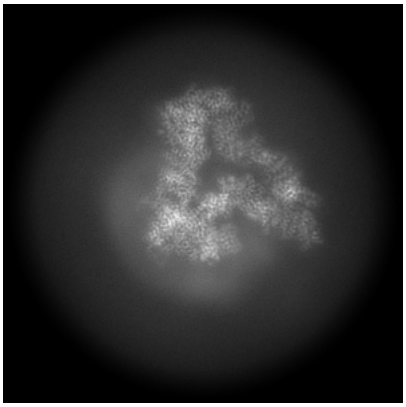
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-73210. These allow visual inspection of the internal detail of the map and identification of artifacts.

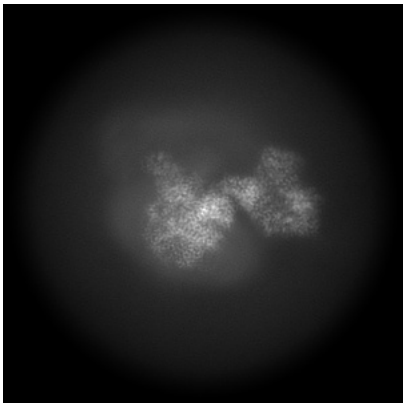
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

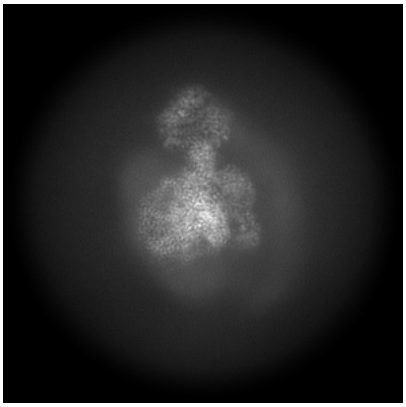
6.1.1 Primary map



X



Y

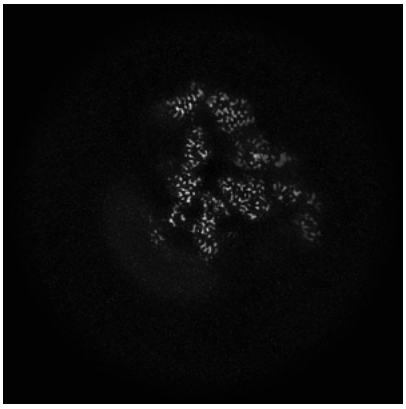


Z

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

6.2 Central slices

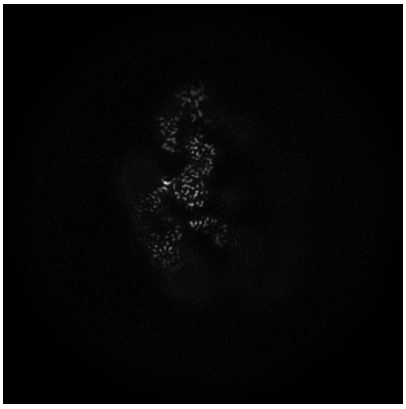
6.2.1 Primary map



X Index: 256



Y Index: 256

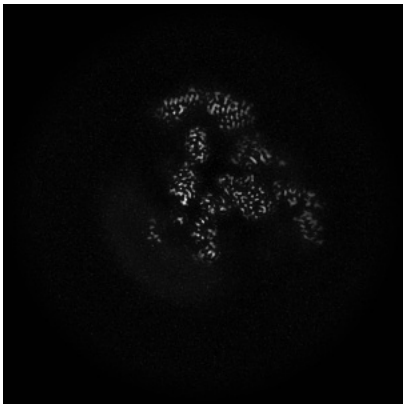


Z Index: 256

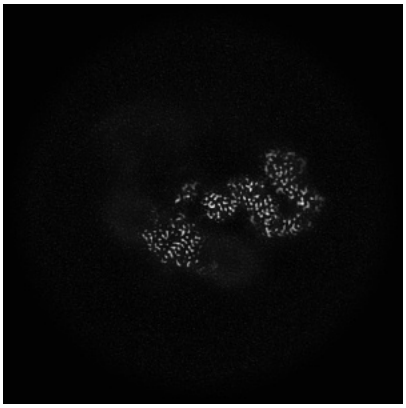
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

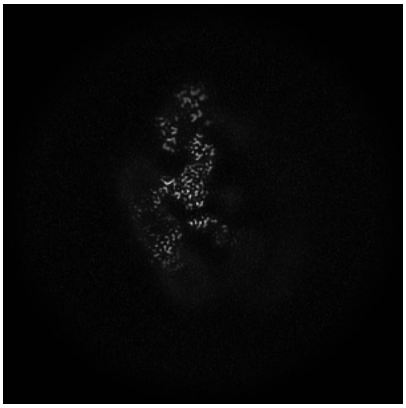
6.3.1 Primary map



X Index: 252



Y Index: 239

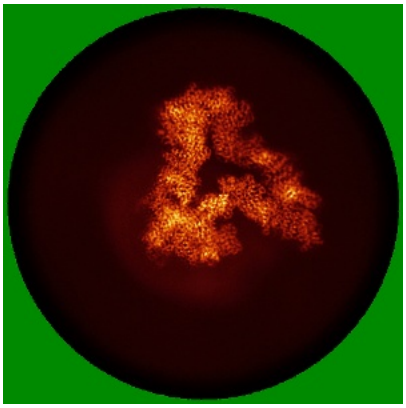


Z Index: 257

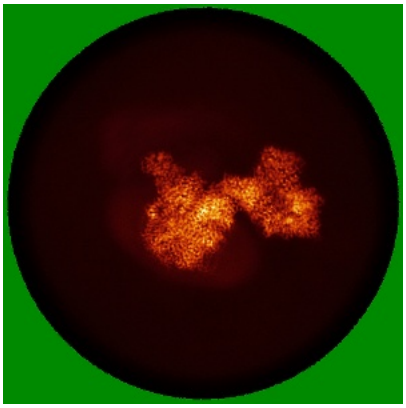
The images above show the largest variance slices of the map in three orthogonal directions.

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

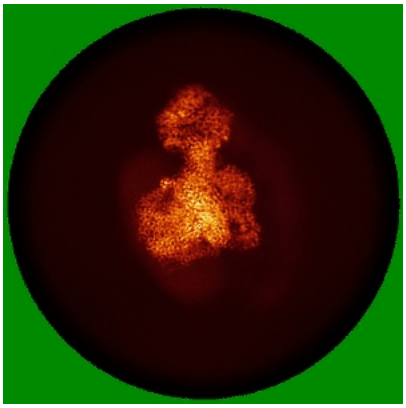
6.4.1 Primary map



X



Y

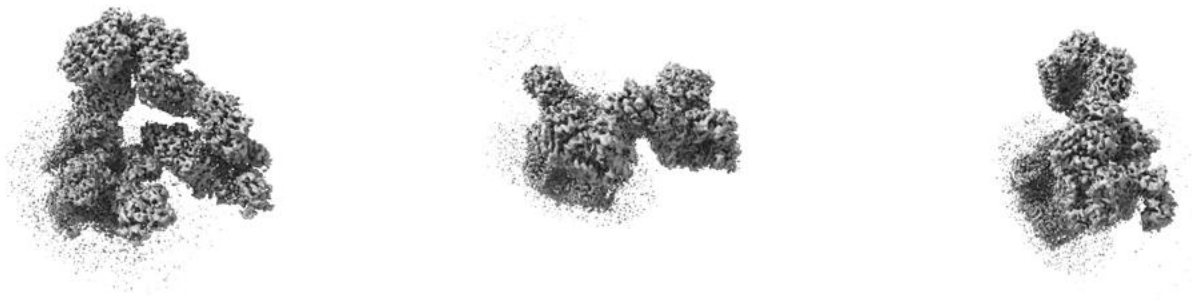


Z

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 0.05. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

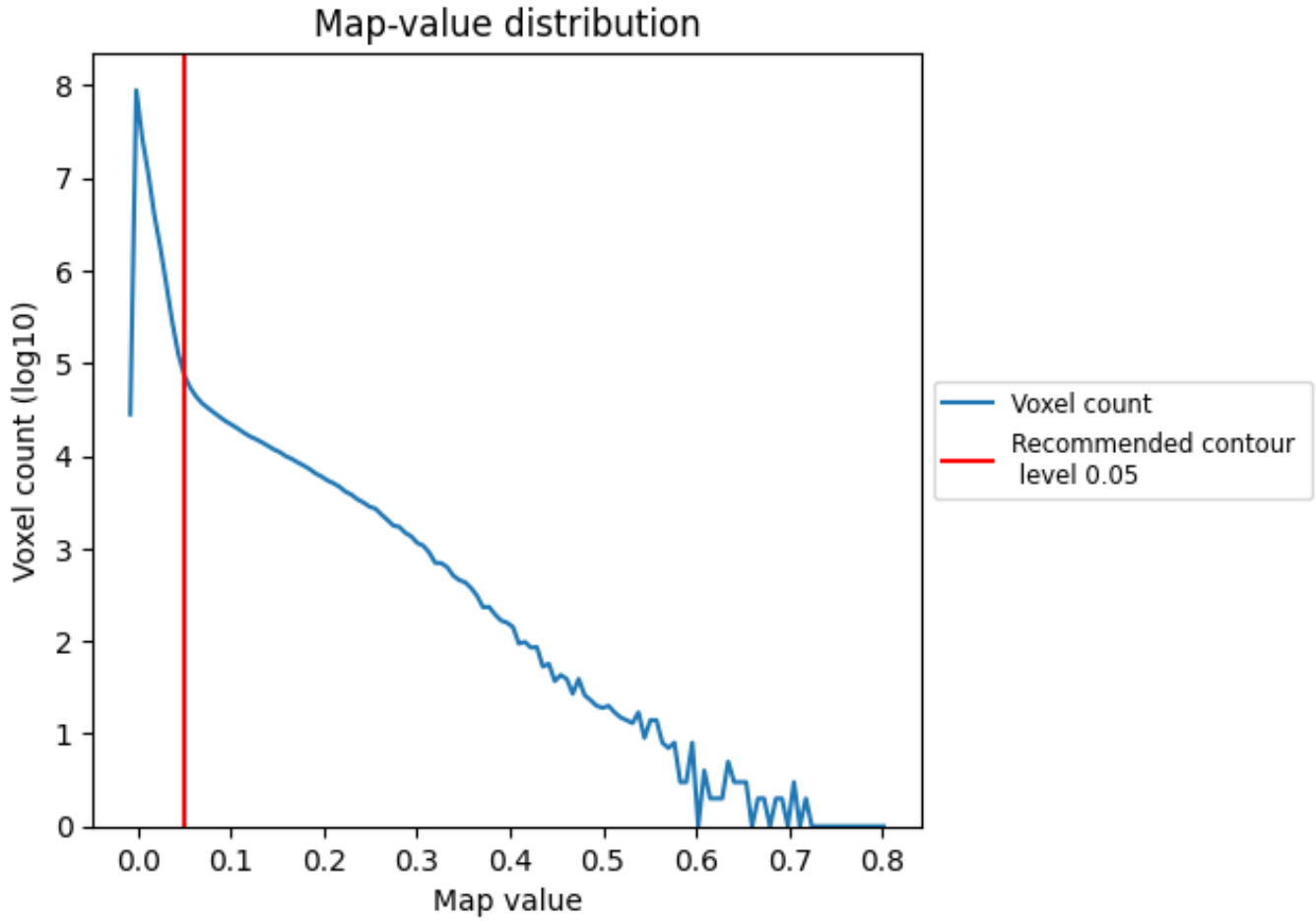
6.6 Mask visualisation (i)

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

7 Map analysis

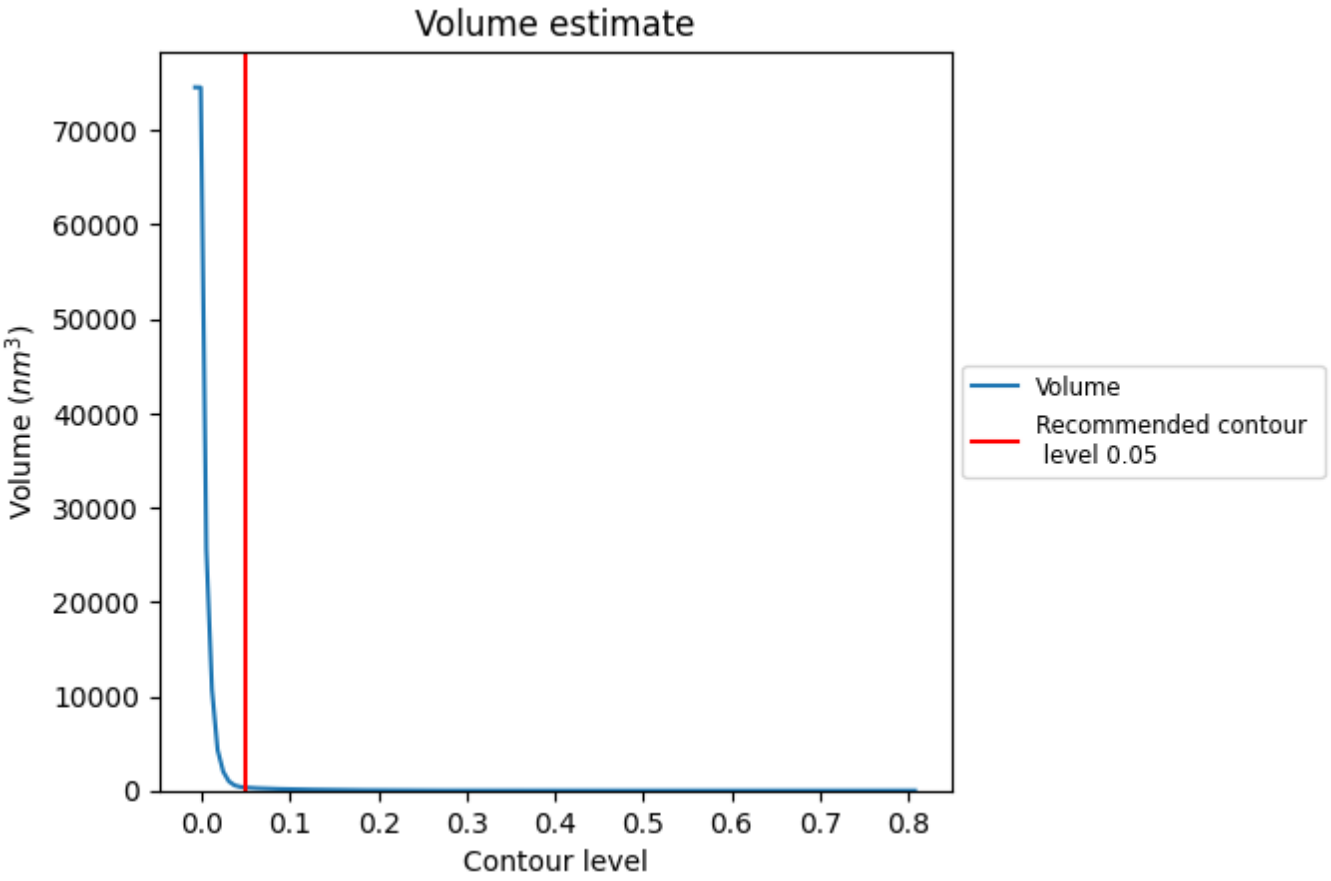
This section contains the results of statistical analysis of the map.

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.

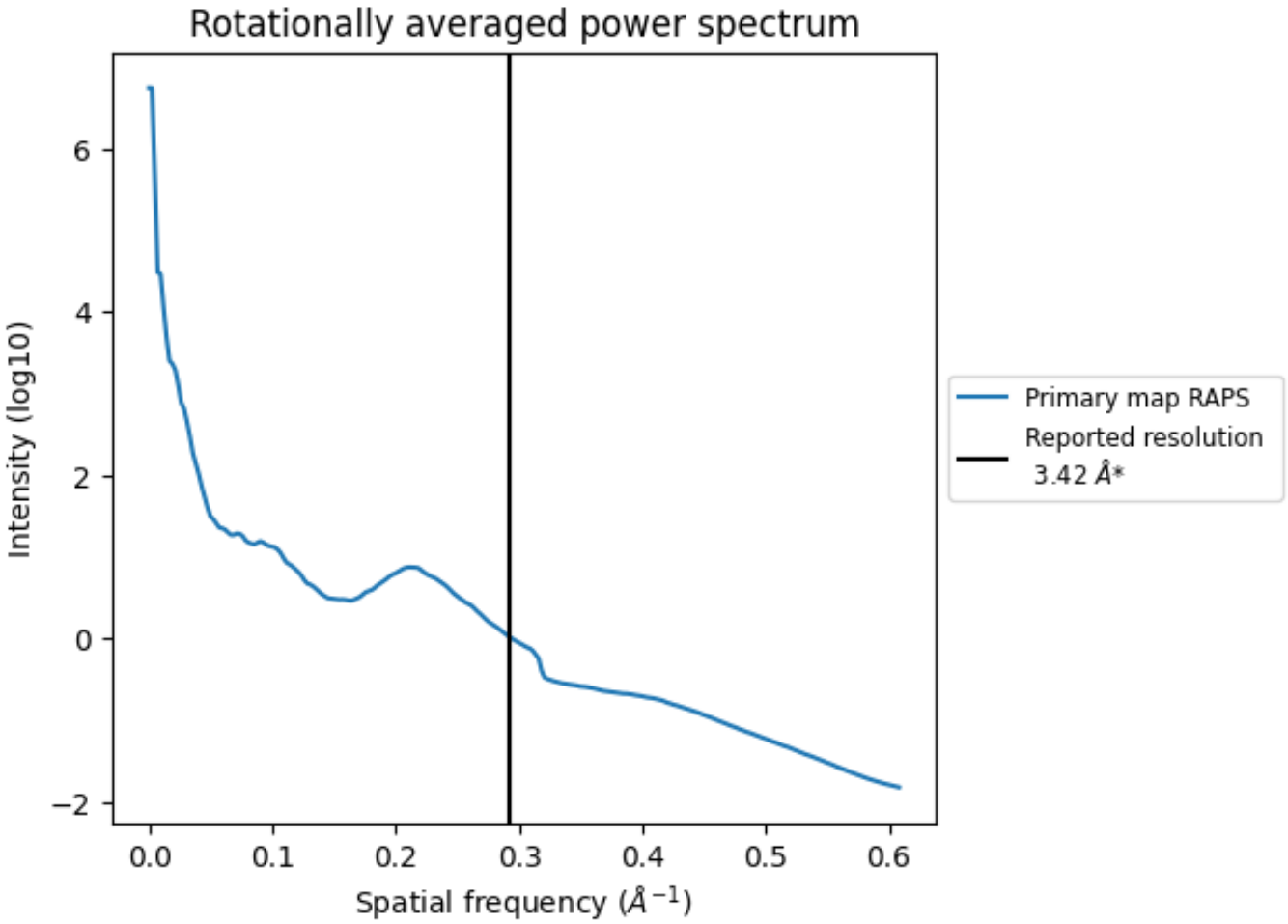
7.2 Volume estimate (i)



The volume at the recommended contour level is 319 nm^3; this corresponds to an approximate mass of 288 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 0.292 Å^{-1}

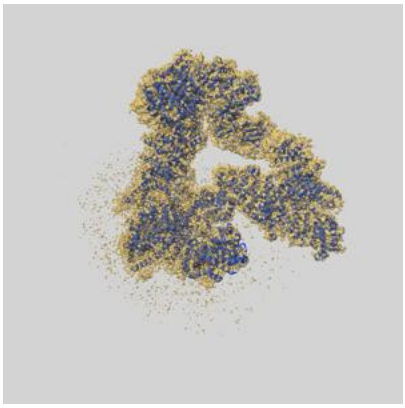
8 Fourier-Shell correlation (i)

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

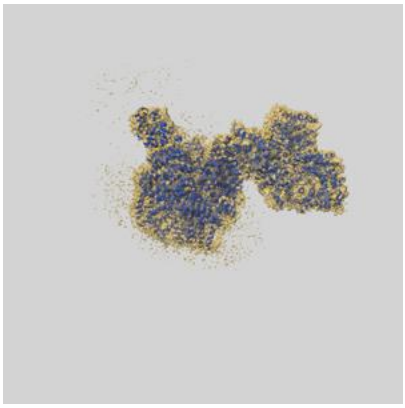
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-73210 and PDB model 9YNK. Per-residue inclusion information can be found in section 3 on page 10.

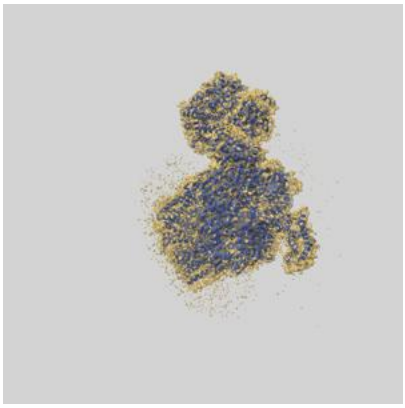
9.1 Map-model overlay



X



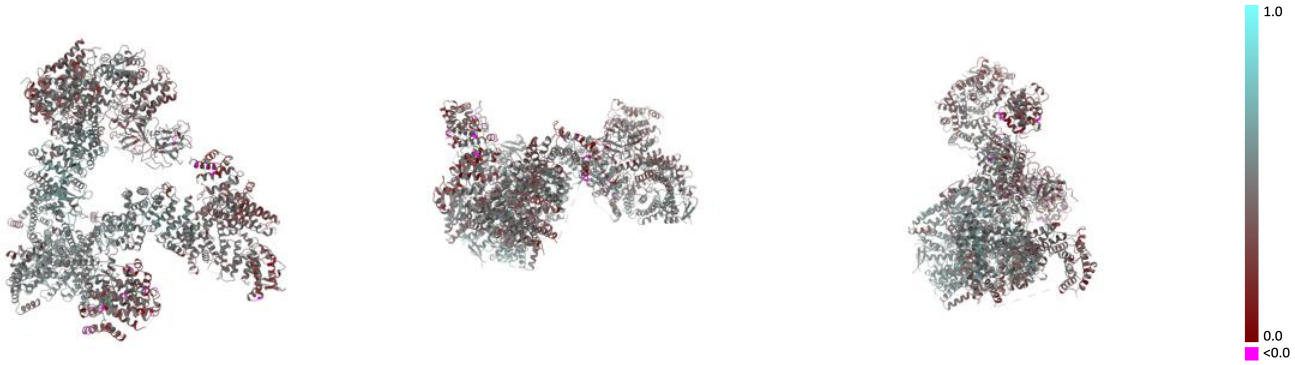
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.05 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.

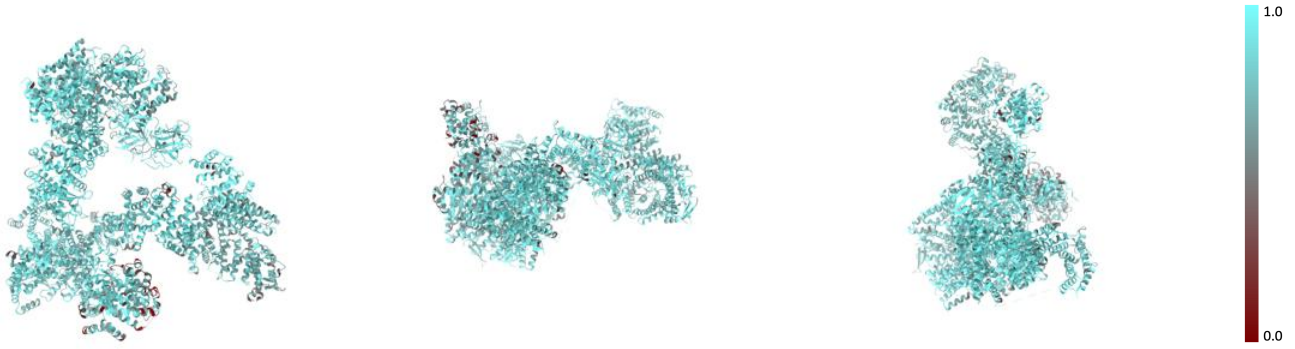
9.2 Q-score mapped to coordinate model



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.

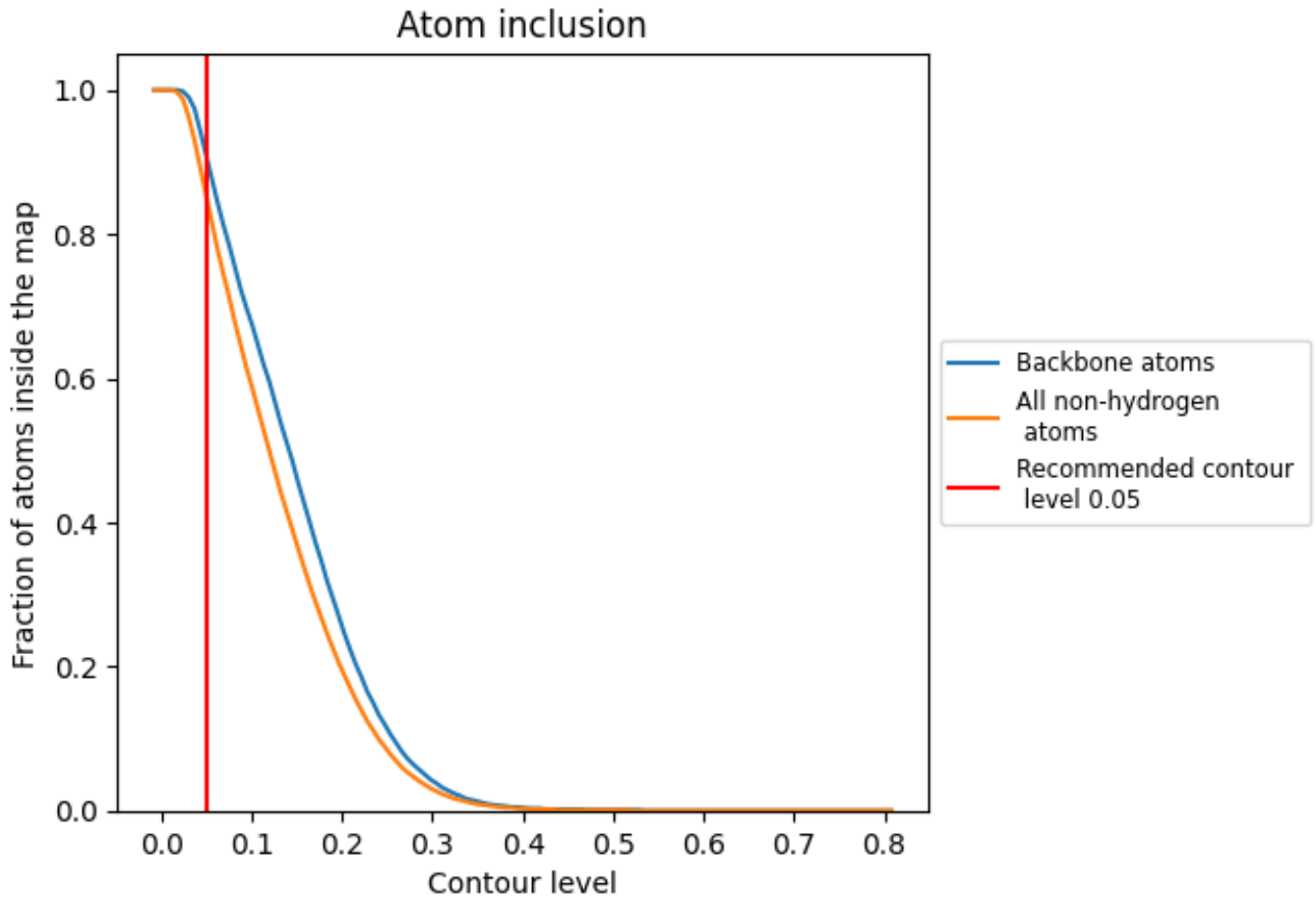
9.3 Atom inclusion mapped to coordinate model



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 (0.05).

9.4 Atom inclusion (i)



At the recommended contour level, 91% of all backbone atoms, 85% 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 (0.05) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.8510	0.4610
A	0.8700	0.4690
B	0.8440	0.4490
C	0.7990	0.4340
D	0.8770	0.5090