Full wwPDB EM Validation Report ⓘ

Aug 8, 2026 – 02:17 PM EDT

PDB ID	:	9YMZ / pdb_00009ymz
EMDB ID	:	EMD-73129
Title	:	Human type 2 IP3 receptor in the inactive-like state (IP3/ATP)
Authors	:	Liu, C.; Lan, Y.; Tang, Q.; Karakas, E.
Deposited on	:	2025-10-10
Resolution	:	3.14 Å(reported)

This is a Full wwPDB EM Validation 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:

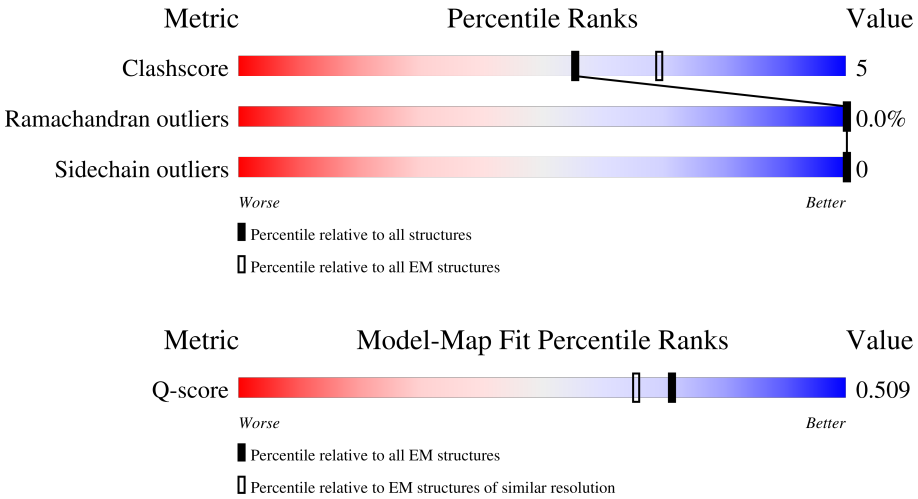
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

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

The reported resolution of this entry is 3.14 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	14483 (2.64 - 3.64)

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% 11% 23%
1	B	2745	48% 8% 44%
1	C	2745	21% 77%
1	D	2745	13% 85%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 38034 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	2112	Total 16945	C 10843	N 2904	O 3096	S 102	0	0
1	B	1547	Total 12417	C 7973	N 2107	O 2256	S 81	0	0
1	C	625	Total 5107	C 3311	N 859	O 903	S 34	0	0
1	D	416	Total 3413	C 2239	N 561	O 594	S 19	0	0

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

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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

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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

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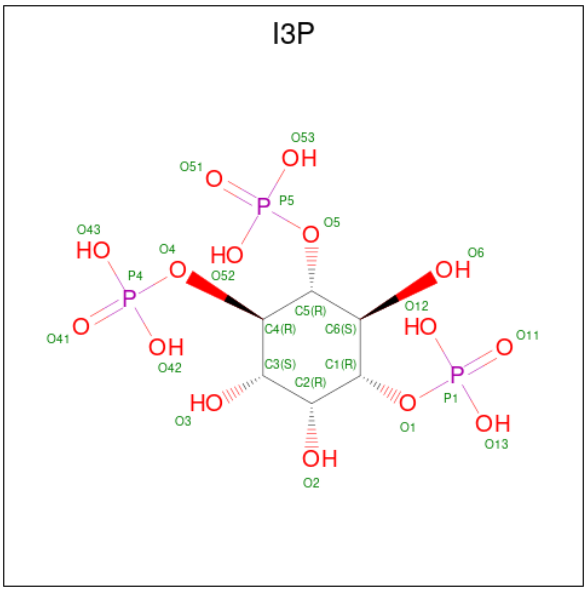
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C	2721	PRO	-	expression tag	UNP Q14571
C	2722	GLN	-	expression tag	UNP Q14571
C	2723	PHE	-	expression tag	UNP Q14571
C	2724	GLU	-	expression tag	UNP Q14571
C	2725	LYS	-	expression tag	UNP Q14571
C	2726	GLY	-	expression tag	UNP Q14571
C	2727	GLY	-	expression 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

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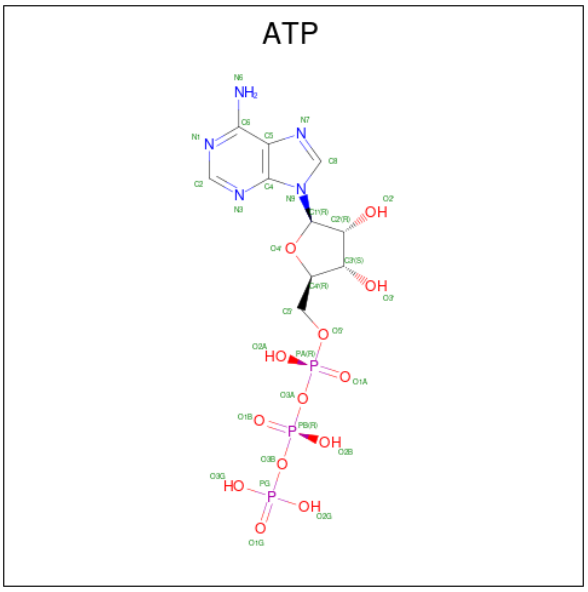
Chain	Residue	Modelled	Actual	Comment	Reference
D	2718	TRP	-	expression tag	UNP Q14571
D	2719	SER	-	expression tag	UNP Q14571
D	2720	HIS	-	expression tag	UNP Q14571
D	2721	PRO	-	expression tag	UNP Q14571
D	2722	GLN	-	expression tag	UNP Q14571
D	2723	PHE	-	expression tag	UNP Q14571
D	2724	GLU	-	expression 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	

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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	

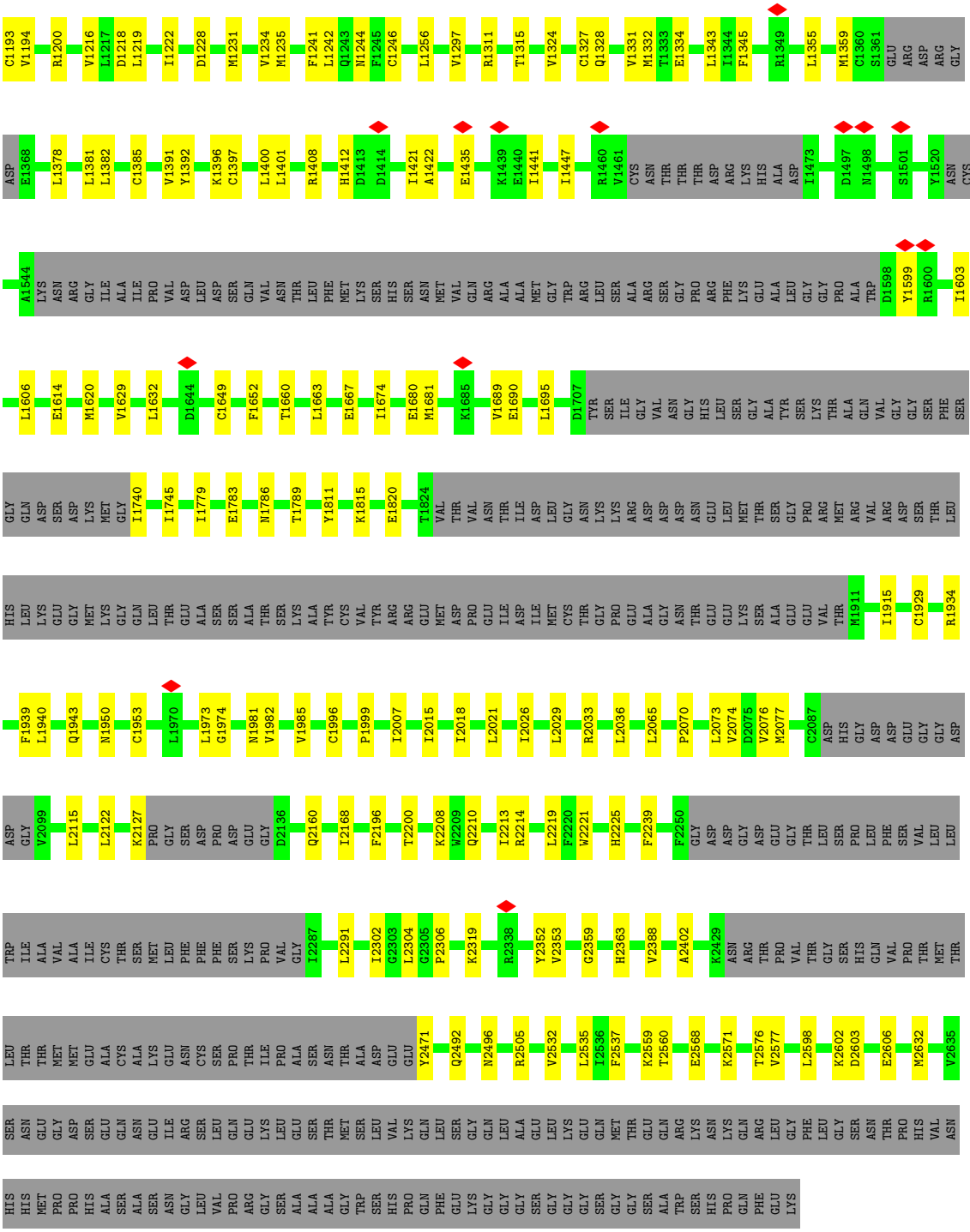
3 Residue-property plots (i)

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

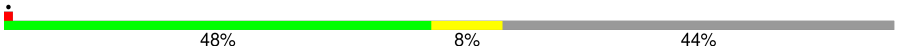
Chain A:

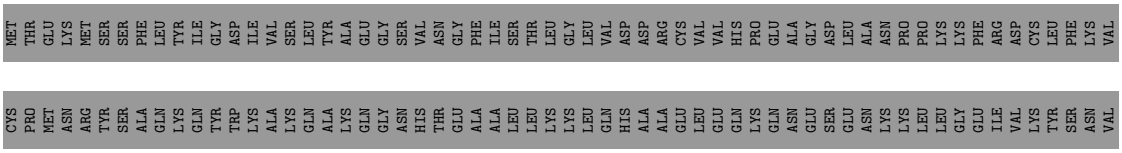


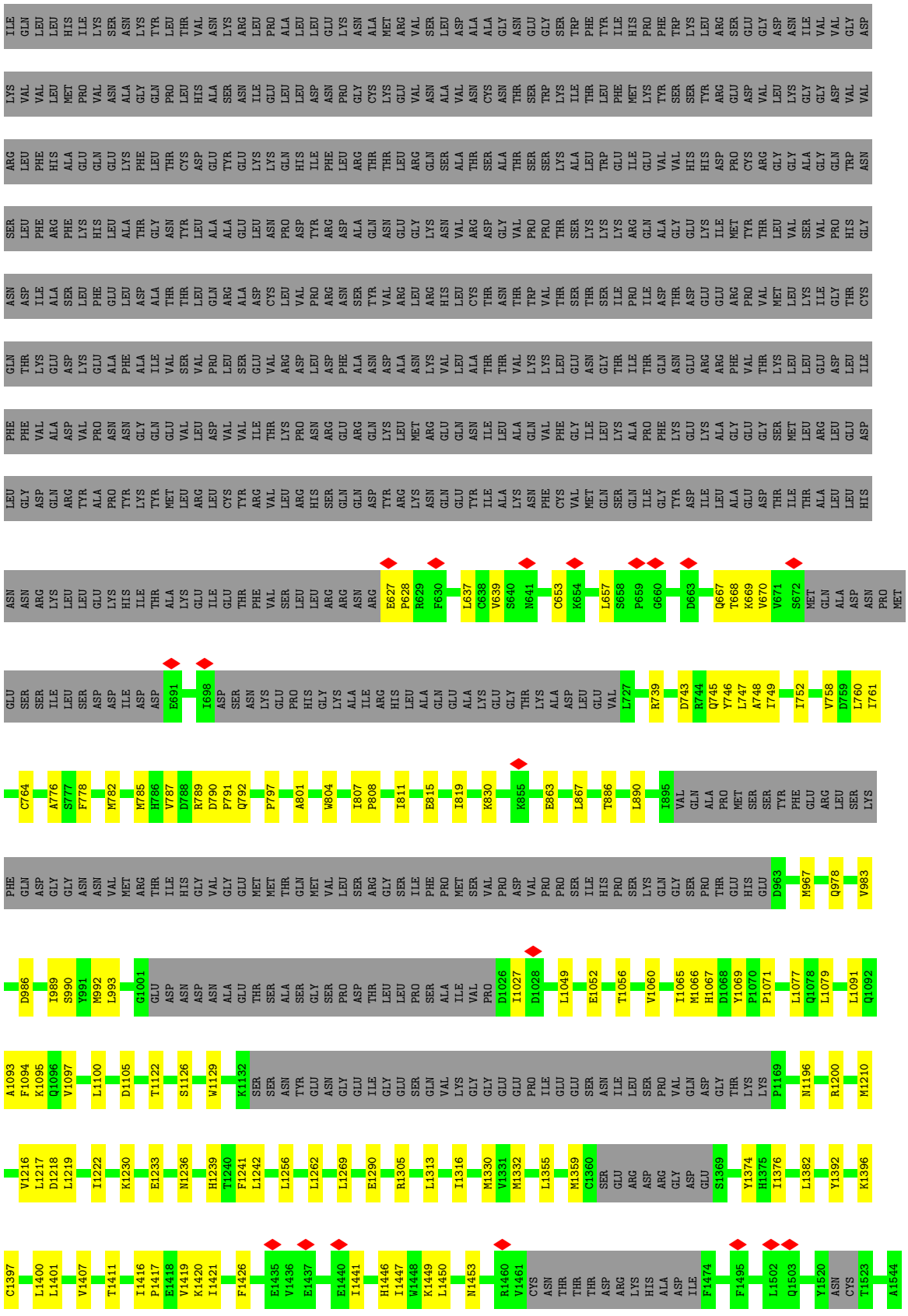


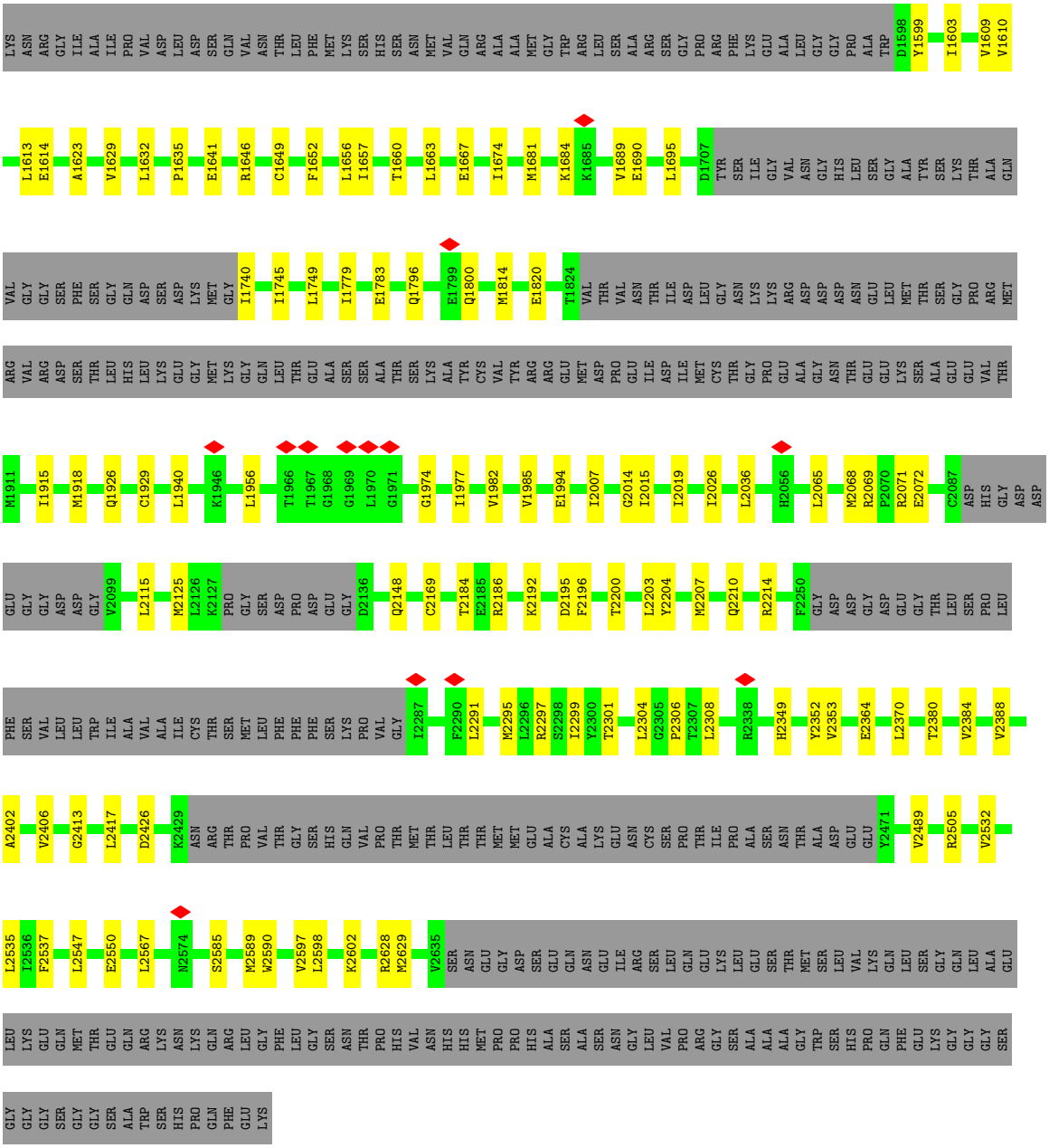
• Molecule 1: Inositol 1,4,5-trisphosphate-gated calcium channel ITPR2

Chain B:





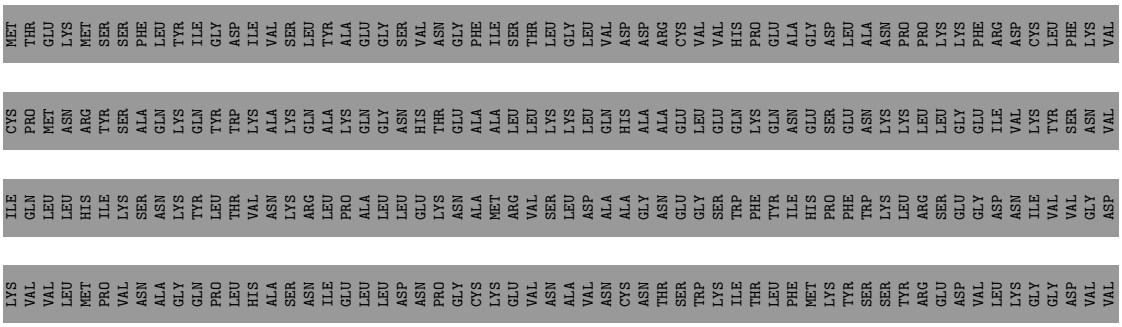


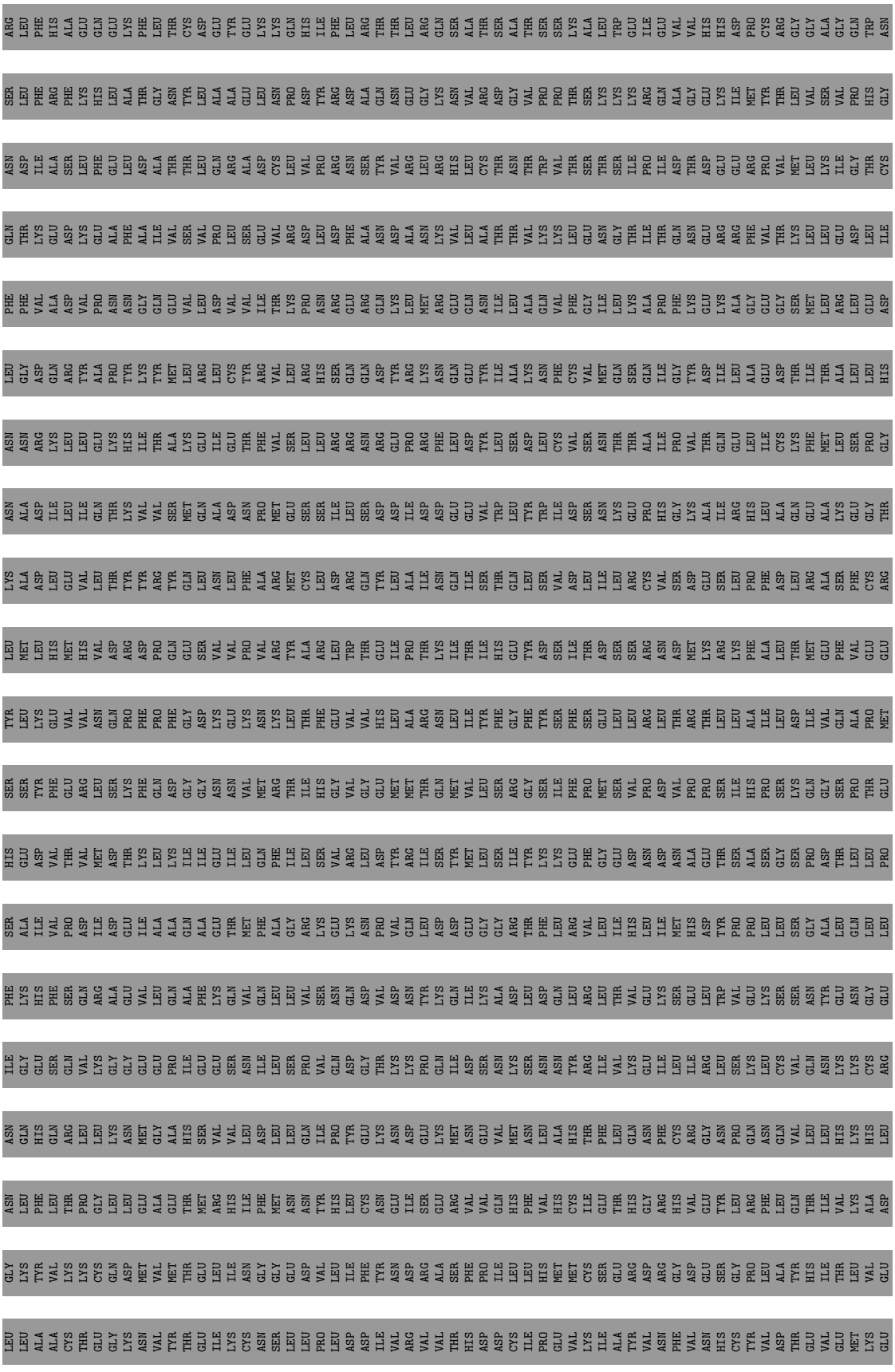


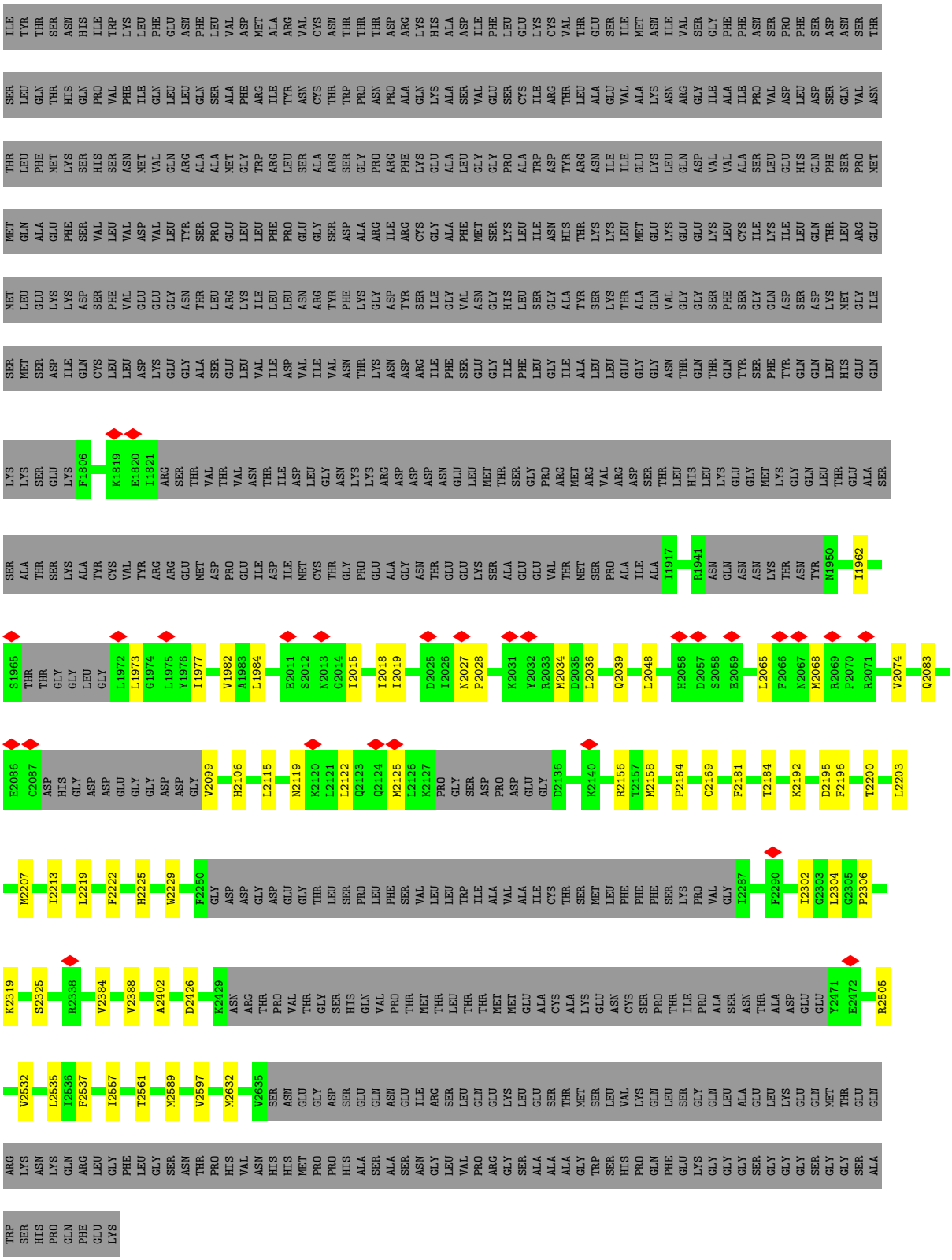
• Molecule 1: Inositol 1,4,5-trisphosphate-gated calcium channel ITPR2

Chain C:





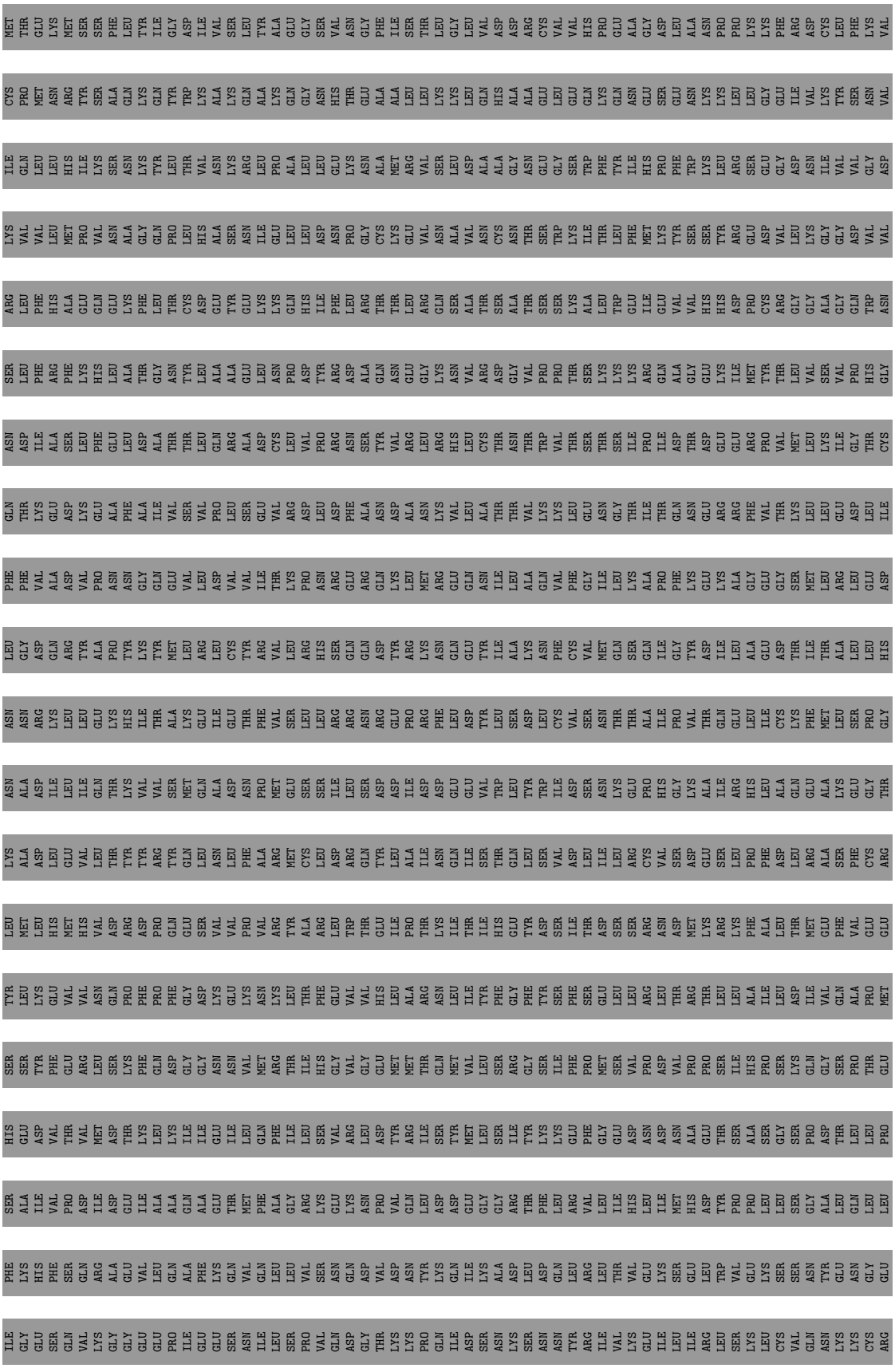


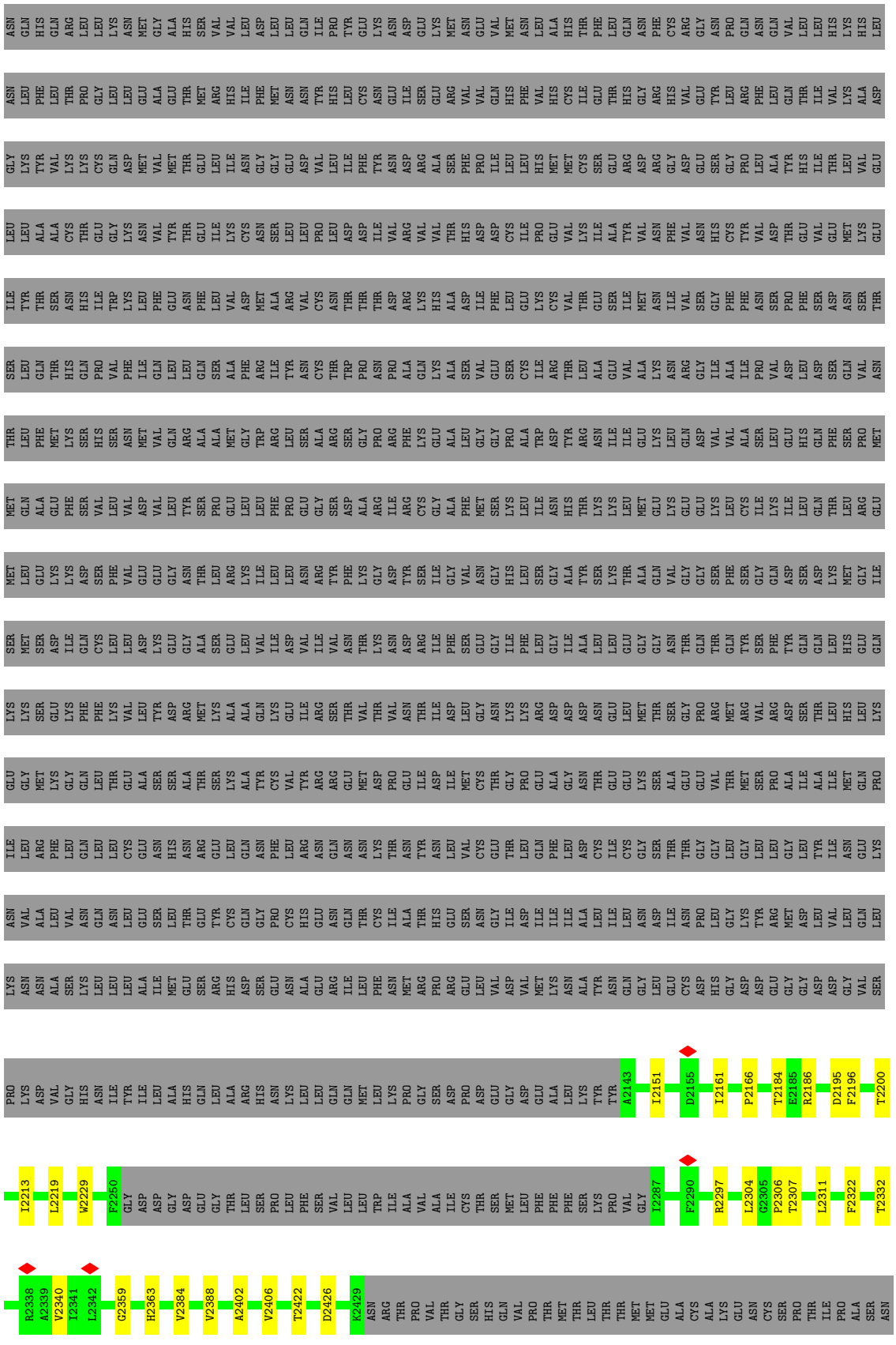


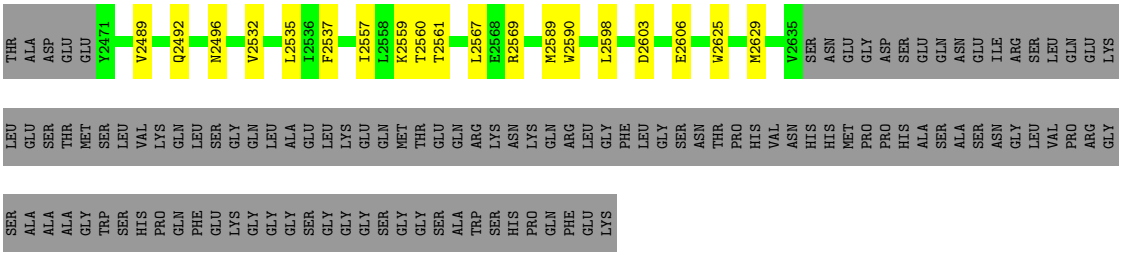
• Molecule 1: Inositol 1,4,5-trisphosphate-gated calcium channel ITPR2

Chain D:




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


A2143
I2151
D2155
I2161
P2166
T2184
E2185
R2186
D2195
F2196
T2200
I2213
L2219
W2229
F2250
I2287
F2290
R2297
L2304
G2305
P2306
T2307
L2311
F2322
T2332
R2338
A2339
V2340
I2341
L2342
G2359
H2363
V2384
V2388
A2402
V2406
T2422
D2426
K2429


THR ALA ASP GLU GLU Y2471 V2489 Q2492 N2496 V2532 L2535 I2536 F2537 I2557 L2558 K2559 T2560 T2561 L2567 E2568 R2569 M2589 W2590 L2598 D2603 E2606 W2625 M2629 V2635 SER ASN GLU GLY ASP SER GLU GLN ASN GLU ILE ARG SER LEU GLN GLU LYS
LEU GLU SER THR MET SER LEU VAL LYS GLN LEU SER GLY GLN LEU ALA GLU LEU LYS GLU GLN MET THR GLU GLN ARG LYS ASN LYS GLN ARG LEU GLY PHE LEU GLY SER ASN THR PRO HIS VAL ASN HIS HIS MET PRO PRO HIS ALA SER ALA SER ASN GLY LEU VAL PRO ARG GLY
SER ALA ALA ALA GLY TRP SER HIS PRO GLN PHE GLU LYS GLY GLY GLY GLY SER GLY GLY GLY SER GLY 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	533134	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	0.627	Depositor
Minimum map value	-0.006	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.010	Depositor
Recommended contour level	0.045	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: ZN, ATP, I3P

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	0.11	0/17254	0.25	0/23315
1	B	0.11	0/12640	0.26	0/17077
1	C	0.10	0/5205	0.23	0/7029
1	D	0.11	0/3490	0.24	0/4723
All	All	0.11	0/38589	0.25	0/52144

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	16945	0	16919	189	0
1	B	12417	0	12367	138	0
1	C	5107	0	5183	39	0
1	D	3413	0	3464	31	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	0	0
3	D	31	0	12	0	0

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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
All	All	38034	0	37990	383	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.

All (383) 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:1926:GLN:HG3	1:B:1994:GLU:HG3	1.63	0.81
1:C:2402:ALA:HB2	1:C:2532:VAL:HG11	1.66	0.77
1:A:2402:ALA:HB2	1:A:2532:VAL:HG11	1.66	0.77
1:A:1099:LEU:HD22	1:A:1606:LEU:HD22	1.69	0.75
1:B:2402:ALA:HB2	1:B:2532:VAL:HG11	1.70	0.74
1:D:2402:ALA:HB2	1:D:2532:VAL:HG11	1.68	0.73
1:A:564:GLN:HB3	1:A:574:ILE:HD12	1.71	0.72
1:A:1982:VAL:HG11	1:A:2036:LEU:HD13	1.72	0.72
1:A:1629:VAL:HG13	1:A:1681:MET:HG2	1.72	0.72
1:B:790:ASP:HB3	1:B:791:PRO:HD3	1.71	0.71
1:A:846:VAL:HG12	1:A:892:ILE:HG13	1.73	0.71
1:A:405:ILE:HD12	1:A:414:MET:HE1	1.75	0.68
1:A:1663:LEU:HD22	1:A:1667:GLU:HB2	1.73	0.68
1:A:761:ILE:HG21	1:A:782:MET:HB2	1.75	0.68
1:A:281:LEU:HD12	1:A:442:LEU:HD13	1.76	0.68
1:A:249:LYS:HE3	1:A:266:THR:HG22	1.78	0.66
1:B:1814:MET:HG2	1:B:1918:MET:HE1	1.78	0.65
1:A:186:PRO:HG2	1:A:189:ALA:HB3	1.77	0.65
1:A:804:TRP:HB2	1:A:1101:VAL:HG12	1.78	0.64
1:A:811:ILE:HG21	1:A:991:TYR:HA	1.80	0.64
1:A:477:GLU:HG3	1:A:493:VAL:HG11	1.80	0.63
1:A:469:ARG:HD3	1:A:548:PRO:HB2	1.80	0.63
1:C:1962:ILE:HD13	1:C:1984:LEU:HD22	1.80	0.62
1:B:797:PRO:HB3	1:B:983:VAL:HG12	1.81	0.62
1:A:1982:VAL:HG21	1:A:2036:LEU:HB3	1.82	0.62
1:A:178:VAL:HG11	1:A:222:LEU:HB2	1.82	0.61
1:B:2186:ARG:HB3	1:B:2192:LYS:HG2	1.81	0.61
1:A:1973:LEU:HD21	1:A:2021:LEU:HD23	1.81	0.61
1:B:2184:THR:HG23	1:B:2195:ASP:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:LEU:HD11	1:A:1106:VAL:HG22	1.83	0.60
1:B:1332:MET:HE1	1:B:1382:LEU:HD22	1.84	0.60
1:A:571:GLN:HE22	1:A:601:ASN:HB2	1.67	0.59
1:B:745:GLN:HG2	1:B:747:LEU:H	1.67	0.59
1:B:1233:GLU:HA	1:B:1236:ASN:HD22	1.68	0.59
1:B:1629:VAL:HG11	1:B:1684:LYS:HD3	1.85	0.58
1:D:2304:LEU:O	1:D:2306:PRO:HD2	2.04	0.58
1:A:298:GLN:HB2	1:A:301:SER:HB3	1.84	0.58
1:C:2304:LEU:O	1:C:2306:PRO:HD2	2.02	0.58
1:C:2537:PHE:HB3	1:D:2537:PHE:HZ	1.68	0.58
1:D:2184:THR:HG23	1:D:2195:ASP:HB3	1.86	0.58
1:A:251:LEU:HG	1:A:262:ILE:HD11	1.85	0.58
1:A:1129:TRP:HA	1:A:1175:LYS:HD3	1.86	0.57
1:B:761:ILE:HG21	1:B:782:MET:HB2	1.85	0.57
1:B:1065:ILE:HG21	1:B:1652:PHE:HE1	1.69	0.57
1:C:2505:ARG:HG3	1:D:2426:ASP:HB2	1.87	0.57
1:C:2207:MET:HE1	1:C:2597:VAL:HG21	1.87	0.57
1:B:978:GLN:HG2	1:B:1079:LEU:HD21	1.86	0.56
1:C:2184:THR:HG23	1:C:2195:ASP:HB3	1.86	0.56
1:B:1417:PRO:HA	1:B:1420:LYS:HB2	1.86	0.56
1:A:525:PRO:HB3	1:A:536:LEU:HD12	1.87	0.56
1:A:1091:LEU:HD21	1:A:1614:GLU:HG2	1.88	0.56
1:D:2213:ILE:HD11	1:D:2219:LEU:HG	1.87	0.56
1:A:603:ARG:HE	1:A:645:ILE:HG12	1.71	0.56
1:A:1228:ASP:HB3	1:A:1231:MET:HB2	1.87	0.56
1:A:38:VAL:HG12	1:A:208:GLU:HA	1.88	0.55
1:A:2304:LEU:O	1:A:2306:PRO:HD2	2.07	0.55
1:B:1977:ILE:HD12	1:B:1985:VAL:HG21	1.87	0.55
1:A:448:ALA:HA	1:A:475:LEU:HD11	1.89	0.55
1:A:882:LEU:HB3	1:A:980:ILE:HG12	1.87	0.55
1:A:1122:THR:HA	1:A:1171:ILE:HD11	1.87	0.55
1:B:1663:LEU:HD22	1:B:1667:GLU:HB2	1.88	0.55
1:A:14:ILE:HG22	1:A:57:LEU:HD12	1.89	0.55
1:A:756:LEU:HD13	1:A:781:LEU:HD21	1.88	0.55
1:B:1242:LEU:HD22	1:B:1256:LEU:HD11	1.87	0.55
1:A:1126:SER:HA	1:A:1129:TRP:NE1	2.22	0.54
1:A:308:LEU:HD21	1:A:439:VAL:HG13	1.88	0.54
1:B:746:TYR:HA	1:B:749:ILE:HB	1.89	0.54
1:B:2304:LEU:O	1:B:2306:PRO:HD2	2.07	0.54
1:B:667:GLN:HB3	1:B:669:LYS:HE3	1.87	0.54
1:A:2319:LYS:HG3	1:A:2353:VAL:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2213:ILE:HD11	1:C:2219:LEU:HG	1.88	0.54
1:B:657:LEU:HD11	1:B:752:ILE:HD11	1.90	0.54
1:C:2535:LEU:HD21	1:D:2388:VAL:HG23	1.90	0.54
1:A:2033:ARG:HE	1:A:2036:LEU:HD11	1.73	0.53
1:A:50:PRO:HD2	1:A:53:PHE:HD1	1.72	0.53
1:C:1982:VAL:HG11	1:C:2036:LEU:HD23	1.89	0.53
1:A:2029:LEU:HD11	1:A:2036:LEU:HD12	1.91	0.52
1:A:241:ARG:HB2	1:A:432:VAL:HB	1.90	0.52
1:A:2505:ARG:HG3	1:B:2426:ASP:HB2	1.90	0.52
1:B:791:PRO:HD2	1:B:792:GLN:NE2	2.24	0.52
1:C:2106:HIS:CE1	1:C:2164:PRO:HB3	2.45	0.52
1:B:789:ARG:HG3	1:B:790:ASP:N	2.25	0.52
1:A:181:LYS:HB3	1:A:217:SER:HB2	1.92	0.52
1:B:1100:LEU:HB3	1:B:1105:ASP:HB3	1.92	0.51
1:A:253:CYS:HB3	1:A:307:HIS:CD2	2.45	0.51
1:A:2537:PHE:HZ	1:D:2537:PHE:HB3	1.75	0.51
1:D:2186:ARG:HH11	1:D:2557:ILE:HD13	1.75	0.51
1:C:2019:ILE:HG22	1:C:2048:LEU:HD11	1.92	0.51
1:B:1230:LYS:O	1:B:1233:GLU:HG2	2.11	0.51
1:B:1407:VAL:HG21	1:B:1446:HIS:HD2	1.75	0.51
1:B:2071:ARG:HB2	1:B:2125:MET:HE1	1.93	0.51
1:A:541:LEU:HD13	1:A:589:ILE:HD11	1.93	0.51
1:A:761:ILE:O	1:A:765:VAL:HG23	2.11	0.51
1:A:2070:PRO:HB3	1:A:2122:LEU:HD13	1.93	0.51
1:A:9:LEU:HB3	1:A:176:ILE:HG23	1.92	0.50
1:A:2319:LYS:HE3	1:A:2352:TYR:CD1	2.46	0.50
1:A:1355:LEU:HG	1:A:1359:MET:HE2	1.94	0.50
1:B:787:VAL:HG21	1:B:867:LEU:HD11	1.93	0.50
1:B:1599:TYR:O	1:B:1603:ILE:HG12	2.10	0.50
1:B:2203:LEU:O	1:B:2207:MET:HG3	2.11	0.50
1:A:2388:VAL:HG23	1:D:2535:LEU:HD21	1.93	0.50
1:A:234:LEU:HB3	1:A:381:VAL:HG13	1.94	0.50
1:D:2196:PHE:O	1:D:2200:THR:HG23	2.11	0.50
1:A:742:LEU:HG	1:A:743:ASP:H	1.77	0.49
1:A:1397:CYS:HA	1:A:1400:LEU:HB2	1.94	0.49
1:A:2535:LEU:HD21	1:B:2388:VAL:HG23	1.92	0.49
1:A:2221:TRP:NE1	1:A:2225:HIS:HE1	2.11	0.49
1:A:2160:GLN:HB2	1:A:2632:MET:HE1	1.93	0.49
1:B:886:THR:HG21	1:B:1049:LEU:HG	1.94	0.49
1:A:2302:ILE:HD12	1:A:2306:PRO:HB2	1.95	0.49
1:A:1324:VAL:HB	1:A:1327:CYS:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:TYR:CE1	1:A:176:ILE:HD13	2.47	0.49
1:B:1239:HIS:CD2	1:B:1269:LEU:HD23	2.48	0.49
1:B:2628:ARG:HD2	1:B:2629:MET:HG2	1.94	0.49
1:D:2304:LEU:HA	1:D:2307:THR:HG22	1.95	0.49
1:A:2074:VAL:HA	1:A:2077:MET:HE2	1.95	0.49
1:A:882:LEU:O	1:A:886:THR:HG23	2.13	0.48
1:A:1242:LEU:HD22	1:A:1256:LEU:HD11	1.94	0.48
1:A:1391:VAL:HB	1:A:1435:GLU:HB3	1.95	0.48
1:B:1091:LEU:HD21	1:B:1614:GLU:HA	1.95	0.48
1:B:2204:TYR:HA	1:B:2207:MET:HE2	1.94	0.48
1:A:134:VAL:HG22	1:A:149:VAL:HG22	1.94	0.48
1:C:2196:PHE:O	1:C:2200:THR:HG23	2.13	0.48
1:A:713:ALA:HA	1:A:727:LEU:HD11	1.94	0.48
1:B:1355:LEU:HG	1:B:1359:MET:HE2	1.94	0.48
1:A:628:PRO:HA	1:A:631:LEU:HD12	1.96	0.48
1:A:2168:ILE:HD11	1:A:2208:LYS:HA	1.96	0.48
1:B:1095:LYS:HG2	1:B:1610:VAL:HG11	1.94	0.48
1:B:1305:ARG:HB3	1:B:1374:TYR:CZ	2.48	0.48
1:B:2148:GLN:HE21	1:B:2585:SER:HB2	1.78	0.48
1:A:787:VAL:HG21	1:A:867:LEU:HD11	1.96	0.48
1:A:640:SER:HB3	1:A:645:ILE:HD11	1.95	0.48
1:A:2492:GLN:O	1:A:2496:ASN:HB2	2.13	0.48
1:B:758:VAL:HG13	1:B:782:MET:HE2	1.95	0.48
1:A:1629:VAL:HG21	1:A:1680:GLU:HG3	1.96	0.48
1:A:2221:TRP:NE1	1:A:2225:HIS:CE1	2.82	0.48
1:A:1441:ILE:HD11	1:A:1447:ILE:HD11	1.95	0.48
1:A:410:GLU:HG3	1:A:411:ARG:H	1.79	0.47
1:C:2065:LEU:HG	1:C:2115:LEU:HD22	1.96	0.47
1:B:2352:TYR:CE1	1:B:2370:LEU:HD22	2.49	0.47
1:A:459:LEU:HG	1:A:464:ILE:HD12	1.95	0.47
1:A:1421:ILE:HG13	1:A:1422:ALA:N	2.29	0.47
1:A:2196:PHE:O	1:A:2200:THR:HG23	2.14	0.47
1:B:653:CYS:SG	1:B:748:ALA:HB2	2.54	0.47
1:B:1660:THR:HA	1:B:1663:LEU:HB2	1.94	0.47
1:B:1956:LEU:HD11	1:B:2014:GLY:HA3	1.97	0.47
1:B:2535:LEU:HD13	1:C:2384:VAL:HG12	1.95	0.47
1:B:2535:LEU:HD21	1:C:2388:VAL:HG23	1.96	0.47
1:A:635:SER:HB2	1:A:739:ARG:HG3	1.95	0.47
1:B:776:ALA:HB1	1:B:863:GLU:HG3	1.96	0.47
1:A:1234:VAL:HG12	1:A:1235:MET:HE2	1.97	0.47
1:B:758:VAL:HG21	1:B:830:LYS:HE3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1216:VAL:HG21	1:B:1241:PHE:CD2	2.49	0.47
1:B:2169:CYS:HA	1:B:2207:MET:SD	2.55	0.47
1:C:2319:LYS:HA	1:C:2319:LYS:HD2	1.69	0.47
1:A:803:LEU:HD23	1:A:806:GLU:HG3	1.97	0.47
1:A:2568:GLU:HB2	1:A:2571:LYS:HD3	1.97	0.47
1:B:815:GLU:O	1:B:819:ILE:HG12	2.14	0.47
1:B:1641:GLU:HA	1:B:1646:ARG:HD3	1.97	0.47
1:B:2184:THR:HG22	1:B:2192:LYS:HB3	1.97	0.47
1:C:2225:HIS:HB3	1:C:2229:TRP:HE1	1.80	0.47
1:D:2492:GLN:O	1:D:2496:ASN:HB2	2.15	0.47
1:A:890:LEU:HD22	1:A:1060:VAL:HG21	1.97	0.47
1:B:1411:THR:HG22	1:B:1453:ASN:HB2	1.96	0.47
1:A:302:LEU:HD23	1:A:366:LEU:HD13	1.96	0.47
1:B:1635:PRO:HG3	1:B:1652:PHE:HD2	1.80	0.47
1:B:639:VAL:HB	1:B:739:ARG:HE	1.79	0.47
1:B:764:CYS:HB3	1:B:778:PHE:CE2	2.50	0.47
1:B:1219:LEU:O	1:B:1222:ILE:HG12	2.15	0.47
1:A:2598:LEU:O	1:A:2602:LYS:HB2	2.15	0.46
1:B:1416:ILE:HG13	1:B:1419:VAL:HG22	1.98	0.46
1:A:240:VAL:HG12	1:A:383:ARG:HH12	1.80	0.46
1:A:745:GLN:HG3	1:A:747:LEU:H	1.79	0.46
1:A:1996:CYS:SG	1:A:2007:ILE:HD12	2.56	0.46
1:A:978:GLN:HG2	1:A:1079:LEU:HD21	1.97	0.46
1:B:2567:LEU:HD23	1:B:2629:MET:HE3	1.97	0.46
1:A:2559:LYS:HG3	1:A:2560:THR:HG23	1.97	0.46
1:B:1635:PRO:HG3	1:B:1652:PHE:CD2	2.51	0.46
1:B:992:MET:HE2	1:B:1613:LEU:HD21	1.98	0.46
1:B:1196:ASN:O	1:B:1200:ARG:HB2	2.15	0.46
1:C:2302:ILE:HD12	1:C:2306:PRO:HB2	1.98	0.46
1:A:1332:MET:HE1	1:A:1382:LEU:HD22	1.98	0.46
1:B:1982:VAL:HG21	1:B:2036:LEU:HB3	1.98	0.46
1:B:2196:PHE:O	1:B:2200:THR:HG23	2.15	0.46
1:A:1740:ILE:HD12	1:A:1745:ILE:HD11	1.96	0.46
1:B:1069:TYR:CD2	1:B:1071:PRO:HD2	2.51	0.46
1:A:838:VAL:HG11	1:A:868:ALA:HB2	1.97	0.46
1:B:2505:ARG:HG3	1:C:2426:ASP:HB2	1.98	0.46
1:A:302:LEU:HB3	1:A:366:LEU:HD22	1.98	0.46
1:A:1216:VAL:HG21	1:A:1241:PHE:CD2	2.51	0.46
1:A:1332:MET:HG3	1:A:1396:LYS:HE2	1.97	0.46
1:B:670:VAL:HG23	1:B:760:LEU:HD12	1.97	0.46
1:B:1392:TYR:O	1:B:1396:LYS:HG3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2169:CYS:HA	1:C:2207:MET:SD	2.56	0.46
1:A:518:VAL:HG13	1:A:556:CYS:HB3	1.98	0.45
1:A:797:PRO:HB3	1:A:983:VAL:HG12	1.98	0.45
1:A:1193:CYS:O	1:A:1200:ARG:HG3	2.15	0.45
1:B:1066:MET:HE1	1:B:1649:CYS:SG	2.56	0.45
1:B:1657:ILE:HA	1:B:1660:THR:HG22	1.98	0.45
1:A:435:PRO:O	1:A:439:VAL:HG23	2.17	0.45
1:A:2073:LEU:O	1:A:2076:VAL:HG12	2.16	0.45
1:B:1974:GLY:HA2	1:B:2026:ILE:HG23	1.98	0.45
1:B:2207:MET:HE1	1:B:2597:VAL:HG21	1.98	0.45
1:A:58:PHE:HB3	1:A:123:LEU:HD12	1.99	0.45
1:A:2535:LEU:HD13	1:B:2384:VAL:HG12	1.99	0.45
1:C:1977:ILE:HD11	1:C:1982:VAL:HA	1.99	0.45
1:A:242:LEU:HD12	1:A:251:LEU:HD23	1.99	0.45
1:A:15:VAL:HG12	1:A:222:LEU:HA	1.99	0.45
1:A:1066:MET:SD	1:A:1649:CYS:HA	2.57	0.45
1:B:2547:LEU:O	1:B:2550:GLU:HG3	2.17	0.45
1:B:986:ASP:HA	1:B:989:ILE:HD12	1.99	0.45
1:B:1401:LEU:HD23	1:B:1426:PHE:CE2	2.51	0.45
1:D:2559:LYS:HA	1:D:2559:LYS:HD3	1.79	0.45
1:A:247:GLN:HB3	1:A:249:LYS:HD2	1.98	0.45
1:C:2119:ASN:HB3	1:C:2122:LEU:HB3	1.99	0.45
1:D:2229:TRP:HB2	1:D:2322:PHE:HD2	1.82	0.45
1:D:2332:THR:HG22	1:D:2340:VAL:HG22	1.97	0.45
1:A:2015:ILE:HA	1:A:2018:ILE:HD12	1.99	0.45
1:A:2033:ARG:HH21	1:A:2036:LEU:HD21	1.82	0.45
1:D:2603:ASP:HB3	1:D:2606:GLU:OE1	2.17	0.45
1:A:758:VAL:HG21	1:A:830:LYS:HE2	1.99	0.45
1:A:1660:THR:OG1	1:A:1674:ILE:HG21	2.16	0.45
1:B:1449:LYS:HA	1:B:1449:LYS:HD3	1.76	0.45
1:C:2015:ILE:HA	1:C:2018:ILE:HD12	1.99	0.45
1:A:602:ASN:HB3	1:A:605:LEU:HB2	1.99	0.44
1:A:2213:ILE:HD11	1:A:2219:LEU:HG	1.99	0.44
1:B:1052:GLU:HB2	1:B:1056:THR:HG23	1.99	0.44
1:A:352:TYR:HB2	1:A:419:THR:OG1	2.17	0.44
1:B:2598:LEU:O	1:B:2602:LYS:HB2	2.18	0.44
1:D:2589:MET:HE3	1:D:2590:TRP:CZ2	2.52	0.44
1:A:1094:PHE:O	1:A:1097:VAL:HG22	2.17	0.44
1:A:653:CYS:SG	1:A:748:ALA:HB2	2.58	0.44
1:A:8:PHE:HB2	1:A:176:ILE:O	2.18	0.44
1:A:1331:VAL:HG11	1:A:1381:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1681:MET:HE2	1:B:1749:LEU:HD11	1.99	0.44
1:B:1689:VAL:HG22	1:B:1690:GLU:H	1.82	0.44
1:A:1689:VAL:HG22	1:A:1690:GLU:H	1.83	0.44
1:B:2413:GLY:HA2	1:B:2417:LEU:HB2	2.00	0.44
1:D:2589:MET:HE3	1:D:2590:TRP:CE2	2.53	0.44
1:A:1219:LEU:O	1:A:1222:ILE:HG12	2.18	0.44
1:B:1217:LEU:HD22	1:B:1262:LEU:HD12	1.99	0.44
1:A:1620:MET:HE3	1:A:1695:LEU:HD22	2.00	0.44
1:A:1934:ARG:NH2	1:A:1999:PRO:HD2	2.32	0.44
1:B:804:TRP:HA	1:B:807:ILE:HD12	2.00	0.44
1:B:1779:ILE:O	1:B:1783:GLU:HG2	2.18	0.44
1:C:1973:LEU:O	1:C:1977:ILE:HG22	2.17	0.44
1:B:1313:LEU:HA	1:B:1316:ILE:HG12	2.00	0.43
1:B:1982:VAL:HG11	1:B:2036:LEU:HD13	2.00	0.43
1:A:58:PHE:HD2	1:A:123:LEU:HB3	1.82	0.43
1:C:2034:MET:HE2	1:C:2083:GLN:HE22	1.84	0.43
1:A:455:THR:HG21	1:A:472:VAL:HB	2.00	0.43
1:A:2239:PHE:HD2	1:A:2291:LEU:HD22	1.83	0.43
1:B:789:ARG:HG3	1:B:790:ASP:H	1.82	0.43
1:B:1820:GLU:HB3	1:B:1915:ILE:HD11	2.00	0.43
1:B:2308:LEU:HD21	1:B:2364:GLU:HG2	1.98	0.43
1:C:2184:THR:HG22	1:C:2192:LYS:HB3	1.99	0.43
1:A:14:ILE:HD13	1:A:224:MET:HB3	2.00	0.43
1:A:2576:THR:HG23	1:A:2577:VAL:HG23	2.01	0.43
1:C:2203:LEU:O	1:C:2207:MET:HG3	2.19	0.43
1:A:1599:TYR:O	1:A:1603:ILE:HG12	2.18	0.43
1:B:1236:ASN:OD1	1:B:1269:LEU:HD21	2.17	0.43
1:B:1610:VAL:O	1:B:1614:GLU:HG3	2.18	0.43
1:B:1632:LEU:HD13	1:B:1652:PHE:CE2	2.53	0.43
1:D:2406:VAL:HG13	1:D:2489:VAL:HG12	2.00	0.43
1:A:1974:GLY:HA2	1:A:2026:ILE:HG23	1.99	0.43
1:B:811:ILE:HD13	1:B:990:SER:HB3	2.00	0.43
1:D:2625:TRP:CD1	1:D:2625:TRP:H	2.37	0.43
1:A:639:VAL:HG22	1:A:644:ALA:HA	2.00	0.43
1:A:2127:LYS:HD3	1:A:2127:LYS:HA	1.85	0.43
1:B:808:PRO:HD2	1:B:811:ILE:HD11	2.00	0.43
1:B:1218:ASP:O	1:B:1222:ILE:HG23	2.18	0.43
1:B:2589:MET:HE3	1:B:2590:TRP:NE1	2.34	0.43
1:D:2359:GLY:HA2	1:D:2363:HIS:O	2.19	0.43
1:B:1740:ILE:HD12	1:B:1745:ILE:HD11	2.01	0.43
1:C:2039:GLN:HE22	1:C:2099:VAL:HB	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2222:PHE:O	1:C:2325:SER:HB2	2.18	0.43
1:D:2567:LEU:HG	1:D:2629:MET:HA	2.01	0.43
1:A:304:ARG:HG2	1:A:365:SER:O	2.18	0.43
1:A:518:VAL:O	1:A:521:ILE:HG22	2.19	0.43
1:A:2239:PHE:CD2	1:A:2291:LEU:HD22	2.54	0.43
1:B:993:LEU:HG	1:B:1094:PHE:HE1	1.83	0.43
1:B:1126:SER:HA	1:B:1129:TRP:CE2	2.54	0.43
1:D:2151:ILE:HD13	1:D:2161:ILE:HD11	2.01	0.43
1:A:1392:TYR:O	1:A:1396:LYS:HG3	2.19	0.43
1:A:2603:ASP:HB3	1:A:2606:GLU:OE1	2.19	0.43
1:B:785:MET:O	1:B:789:ARG:HD2	2.18	0.43
1:A:585:ILE:HD11	1:A:592:GLU:HG3	2.00	0.42
1:A:670:VAL:HG23	1:A:760:LEU:HD12	2.01	0.42
1:A:1950:ASN:HB3	1:A:1953:CYS:HB2	2.01	0.42
1:B:1122:THR:HG22	1:B:1129:TRP:CZ2	2.54	0.42
1:B:1290:GLU:HA	1:B:1330:MET:SD	2.59	0.42
1:B:2295:MET:HE2	1:B:2299:ILE:HD11	2.01	0.42
1:A:1343:LEU:HD23	1:A:1378:LEU:HD11	2.01	0.42
1:A:1820:GLU:OE1	1:A:1915:ILE:HD11	2.18	0.42
1:A:2471:TYR:CE2	1:D:2422:THR:HG21	2.54	0.42
1:B:785:MET:HE3	1:B:785:MET:HB2	1.83	0.42
1:B:1077:LEU:HD13	1:B:1674:ILE:HD11	2.01	0.42
1:A:622:LEU:HD21	1:A:631:LEU:HG	2.01	0.42
1:A:1786:ASN:HB3	1:A:1789:THR:OG1	2.20	0.42
1:B:1417:PRO:O	1:B:1421:ILE:HG12	2.19	0.42
1:A:1779:ILE:O	1:A:1783:GLU:HG2	2.19	0.42
1:B:1450:LEU:HD23	1:B:1450:LEU:HA	1.86	0.42
1:A:771:PRO:HB2	1:A:773:ASP:OD1	2.20	0.42
1:B:2069:ARG:HB3	1:B:2072:GLU:HB2	2.01	0.42
1:A:1311:ARG:O	1:A:1315:THR:HG23	2.19	0.42
1:A:1929:CYS:SG	1:A:1940:LEU:HD22	2.60	0.42
1:D:2557:ILE:O	1:D:2561:THR:HB	2.20	0.42
1:A:1193:CYS:HB3	1:A:1244:ASN:HB3	2.02	0.42
1:B:1397:CYS:HA	1:B:1400:LEU:HB2	2.01	0.42
1:B:2349:HIS:O	1:B:2353:VAL:HG23	2.20	0.42
1:D:2297:ARG:HD2	1:D:2297:ARG:HA	1.75	0.42
1:A:115:VAL:O	1:A:176:ILE:HG22	2.20	0.42
1:B:1093:ALA:O	1:B:1097:VAL:HG13	2.20	0.42
1:B:2210:GLN:O	1:B:2214:ARG:HG2	2.20	0.42
1:A:363:ILE:HD12	1:A:366:LEU:HD12	2.02	0.41
1:A:1058:LEU:O	1:A:1062:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1297:VAL:HG21	1:A:1334:GLU:HB3	2.01	0.41
1:A:1981:ASN:O	1:A:1985:VAL:HG23	2.19	0.41
1:B:801:ALA:HB3	1:B:1210:MET:HE3	2.01	0.41
1:B:1441:ILE:HD11	1:B:1447:ILE:HD11	2.02	0.41
1:D:2311:LEU:HD23	1:D:2311:LEU:HA	1.87	0.41
1:A:837:PHE:O	1:A:840:GLU:HG3	2.19	0.41
1:A:1093:ALA:O	1:A:1097:VAL:HG13	2.20	0.41
1:A:1408:ARG:O	1:A:1412:HIS:HB2	2.19	0.41
1:C:2027:ASN:HB2	1:C:2028:PRO:HD3	2.01	0.41
1:A:166:PHE:HE1	1:A:215:ASN:HB2	1.85	0.41
1:A:168:LYS:HE2	1:A:168:LYS:HB3	1.88	0.41
1:A:1401:LEU:HD12	1:A:1401:LEU:HA	1.89	0.41
1:B:1027:ILE:HG22	1:B:1609:VAL:HA	2.02	0.41
1:A:980:ILE:HA	1:A:983:VAL:HG22	2.01	0.41
1:A:2065:LEU:HG	1:A:2115:LEU:HD22	2.02	0.41
1:A:2359:GLY:HA2	1:A:2363:HIS:O	2.20	0.41
1:B:668:THR:HG22	1:B:760:LEU:HD11	2.01	0.41
1:C:2181:PHE:HB2	1:C:2589:MET:HE1	2.03	0.41
1:B:967:MET:HE1	1:B:1067:HIS:CD2	2.55	0.41
1:B:1077:LEU:HD21	1:B:1656:LEU:HD11	2.01	0.41
1:A:1328:GLN:HG2	1:A:1385:CYS:HA	2.03	0.41
1:A:1632:LEU:HD22	1:A:1652:PHE:HE2	1.84	0.41
1:A:1811:TYR:O	1:A:1815:LYS:HG2	2.21	0.41
1:A:2210:GLN:HA	1:A:2213:ILE:HG22	2.02	0.41
1:C:2158:MET:HB3	1:C:2632:MET:HE2	2.02	0.41
1:C:2557:ILE:O	1:C:2561:THR:HB	2.20	0.41
1:A:1190:SER:O	1:A:1194:VAL:HG22	2.20	0.41
1:B:2007:ILE:HG22	1:B:2015:ILE:HD11	2.03	0.41
1:D:2166:PRO:HG3	1:D:2598:LEU:HB2	2.03	0.41
1:A:251:LEU:HD13	1:A:417:ILE:HD13	2.03	0.41
1:A:384:ASN:HA	1:A:431:ILE:O	2.21	0.41
1:A:596:THR:O	1:A:600:HIS:HB2	2.21	0.41
1:A:835:MET:HG2	1:A:871:LEU:HD13	2.03	0.41
1:A:1246:CYS:SG	1:A:1256:LEU:HD12	2.61	0.41
1:A:1345:PHE:HZ	1:A:1382:LEU:HD11	1.86	0.41
1:D:2560:THR:HG22	1:D:2569:ARG:HE	1.85	0.41
1:A:519:PHE:HZ	1:A:574:ILE:HG23	1.85	0.41
1:A:1939:PHE:O	1:A:1943:GLN:HG3	2.21	0.41
1:B:637:LEU:HD23	1:B:637:LEU:HA	1.95	0.41
1:B:890:LEU:HD22	1:B:1060:VAL:HG21	2.02	0.41
1:B:1929:CYS:SG	1:B:1940:LEU:HD22	2.61	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2065:LEU:HG	1:B:2115:LEU:HD22	2.03	0.41
1:B:2297:ARG:HE	1:B:2301:THR:HG21	1.86	0.41
1:C:2535:LEU:HD13	1:D:2384:VAL:HG12	2.03	0.41
1:A:547:ALA:N	1:A:548:PRO:HD2	2.36	0.40
1:A:661:ASN:O	1:A:664:ILE:HG12	2.21	0.40
1:A:1218:ASP:O	1:A:1222:ILE:HG23	2.21	0.40
1:B:1623:ALA:HB3	1:B:1695:LEU:HD23	2.03	0.40
1:A:585:ILE:CD1	1:A:592:GLU:HG3	2.51	0.40
1:A:839:GLU:HG3	1:A:843:LYS:HE2	2.02	0.40
1:A:886:THR:HG22	1:A:980:ILE:HD13	2.02	0.40
1:A:2210:GLN:O	1:A:2214:ARG:HG2	2.21	0.40
1:B:1376:ILE:HG12	1:B:1419:VAL:HG12	2.03	0.40
1:B:2380:THR:O	1:B:2384:VAL:HG23	2.21	0.40
1:A:707:LYS:HG2	1:A:712:LEU:HG	2.03	0.40
1:B:627:GLU:HA	1:B:628:PRO:HD3	1.97	0.40
1:B:2019:ILE:HG23	1:B:2068:MET:HE3	2.03	0.40
1:B:2291:LEU:HD23	1:B:2291:LEU:HA	1.92	0.40
1:B:2406:VAL:HG13	1:B:2489:VAL:HG12	2.02	0.40
1:B:2537:PHE:HB3	1:C:2537:PHE:HZ	1.86	0.40
1:C:2074:VAL:HG21	1:C:2125:MET:SD	2.61	0.40
1:B:1796:GLN:O	1:B:1800:GLN:HB2	2.21	0.40
1:C:2065:LEU:HD23	1:C:2068:MET:HE3	2.04	0.40
1:C:2156:ARG:HD3	1:C:2156:ARG:HA	1.90	0.40
1:A:239:VAL:HA	1:A:282:TRP:O	2.21	0.40
1:A:239:VAL:HG23	1:A:434:VAL:HB	2.03	0.40
1:A:1632:LEU:HD22	1:A:1652:PHE:CE2	2.57	0.40

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	2072/2745 (76%)	2005 (97%)	67 (3%)	0	100	100
1	B	1515/2745 (55%)	1462 (96%)	52 (3%)	1 (0%)	48	76
1	C	609/2745 (22%)	599 (98%)	10 (2%)	0	100	100
1	D	410/2745 (15%)	402 (98%)	8 (2%)	0	100	100
All	All	4606/10980 (42%)	4468 (97%)	137 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	743	ASP

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	1857/2448 (76%)	1857 (100%)	0	100	100
1	B	1357/2448 (55%)	1357 (100%)	0	100	100
1	C	568/2448 (23%)	568 (100%)	0	100	100
1	D	378/2448 (15%)	378 (100%)	0	100	100
All	All	4160/9792 (42%)	4160 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	122	GLN
1	A	194	HIS
1	A	197	ASN
1	A	784	HIS
1	A	792	GLN
1	A	1083	HIS
1	A	1096	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	1111	GLN
1	A	1195	GLN
1	A	1221	GLN
1	A	1390	ASN
1	A	1796	GLN
1	A	1818	GLN
1	A	2079	ASN
1	A	2194	ASN
1	A	2225	HIS
1	A	2318	ASN
1	A	2588	ASN
1	A	2591	HIS
1	B	750	ASN
1	B	792	GLN
1	B	1033	GLN
1	B	1111	GLN
1	B	1118	GLN
1	B	1195	GLN
1	B	1209	ASN
1	B	1453	ASN
1	B	1987	GLN
1	B	2027	ASN
1	B	2118	HIS
1	B	2199	GLN
1	B	2329	ASN
1	B	2349	HIS
1	C	2001	HIS
1	C	2083	GLN
1	C	2113	HIS
1	C	2194	ASN
1	C	2199	GLN
1	D	2189	GLN
1	D	2492	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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 9 ligands modelled in this entry, 4 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	A	2802	-	32,33,33	0.28	0	48,52,52	0.31	0
3	ATP	B	2801	-	32,33,33	0.28	0	48,52,52	0.35	0
3	ATP	D	2801	-	32,33,33	0.27	0	48,52,52	0.33	0
3	ATP	C	2801	-	32,33,33	0.28	0	48,52,52	0.32	0
2	I3P	A	2801	-	24,24,24	2.17	3 (12%)	39,39,39	0.86	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	A	2802	-	-	6/22/38/38	0/3/3/3
3	ATP	B	2801	-	-	4/22/38/38	0/3/3/3
3	ATP	D	2801	-	-	4/22/38/38	0/3/3/3
3	ATP	C	2801	-	-	7/22/38/38	0/3/3/3
2	I3P	A	2801	-	-	0/15/39/39	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2801	I3P	P4-O4	6.02	1.70	1.59
2	A	2801	I3P	P5-O5	5.80	1.69	1.59
2	A	2801	I3P	P1-O1	5.70	1.69	1.59

There are no bond angle outliers.

There are no chirality outliers.

All (21) torsion outliers are listed below:

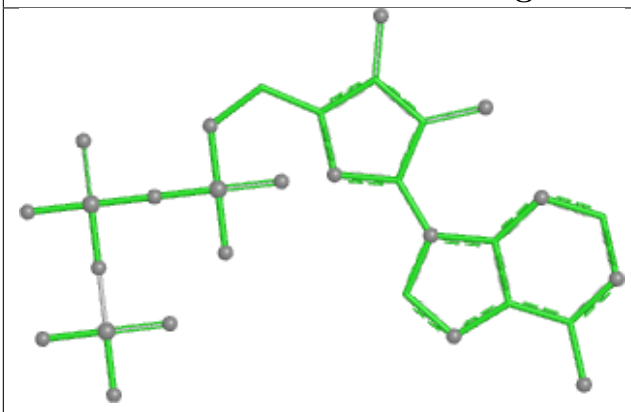
Mol	Chain	Res	Type	Atoms
3	A	2802	ATP	PB-O3B-PG-O2G
3	A	2802	ATP	C5'-O5'-PA-O1A
3	A	2802	ATP	C5'-O5'-PA-O3A
3	C	2801	ATP	PB-O3B-PG-O2G
3	C	2801	ATP	C5'-O5'-PA-O1A
3	C	2801	ATP	C5'-O5'-PA-O3A
3	D	2801	ATP	C5'-O5'-PA-O1A
3	B	2801	ATP	PG-O3B-PB-O3A
3	A	2802	ATP	PB-O3A-PA-O5'
3	B	2801	ATP	C5'-O5'-PA-O3A
3	C	2801	ATP	C5'-O5'-PA-O2A
3	A	2802	ATP	PB-O3B-PG-O1G
3	C	2801	ATP	PB-O3B-PG-O1G
3	D	2801	ATP	PB-O3B-PG-O1G
3	D	2801	ATP	PB-O3A-PA-O1A
3	B	2801	ATP	PG-O3B-PB-O2B
3	C	2801	ATP	PB-O3A-PA-O1A
3	C	2801	ATP	PB-O3A-PA-O2A
3	B	2801	ATP	PG-O3B-PB-O1B
3	D	2801	ATP	PB-O3A-PA-O2A
3	A	2802	ATP	O4'-C4'-C5'-O5'

There are no ring outliers.

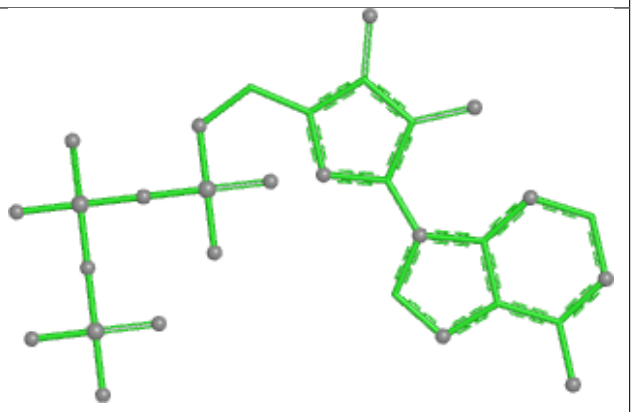
No monomer is involved in short contacts.

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.

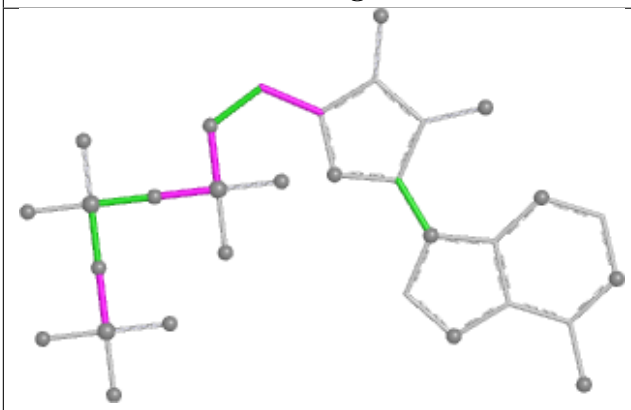
Ligand ATP A 2802



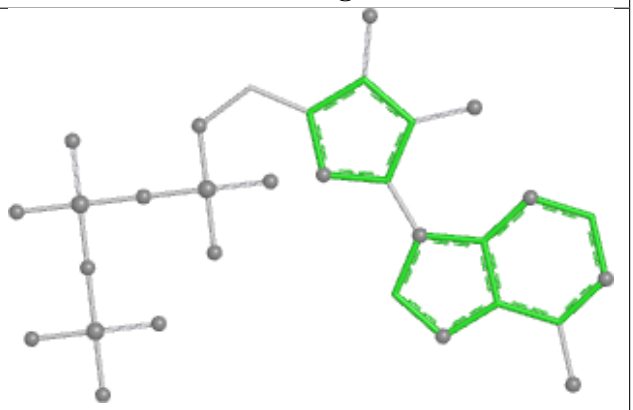
Bond lengths



Bond angles

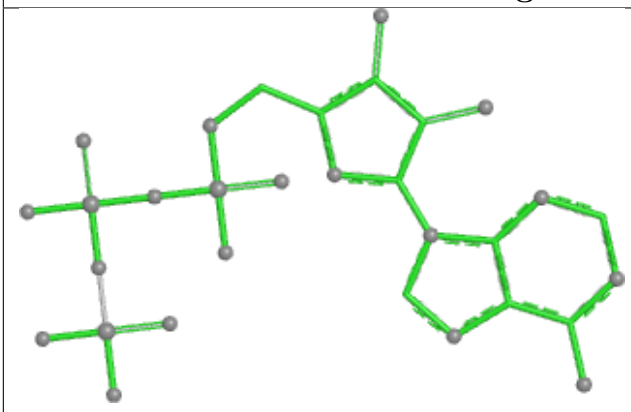


Torsions

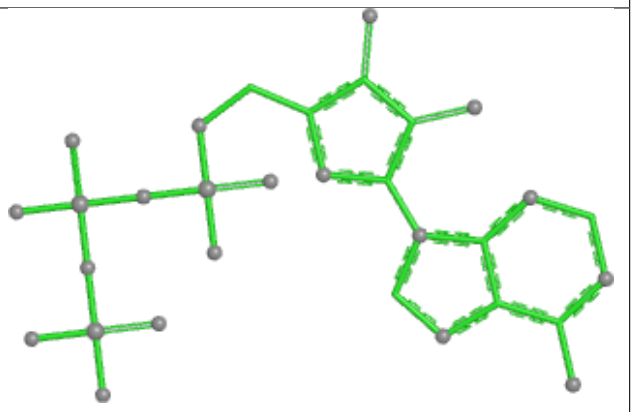


Rings

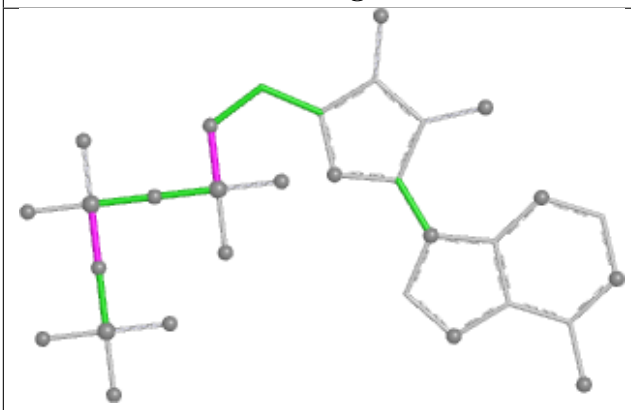
Ligand ATP B 2801



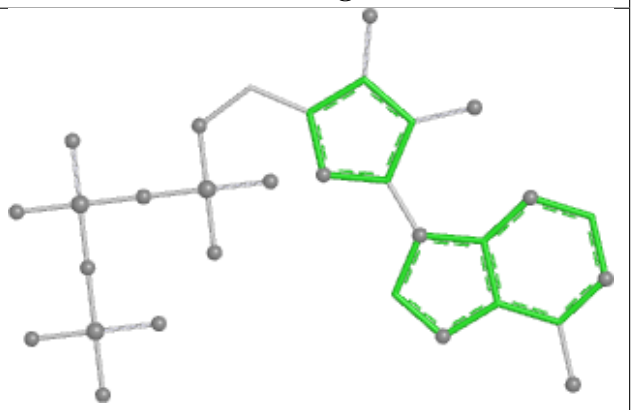
Bond lengths



Bond angles

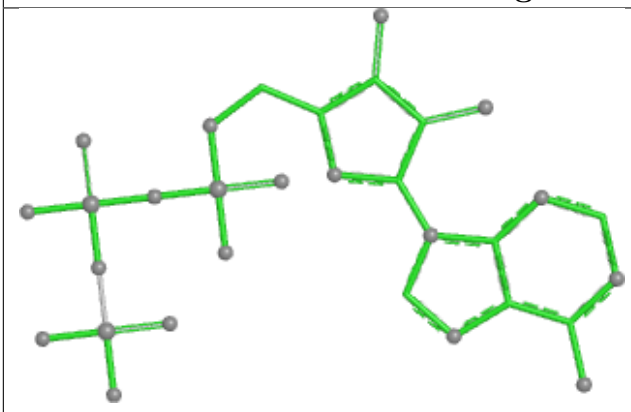


Torsions

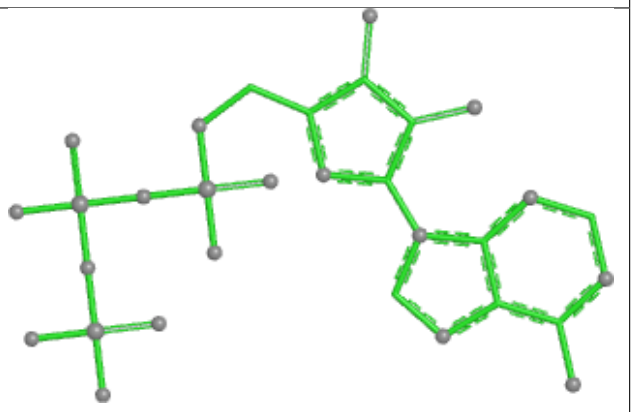


Rings

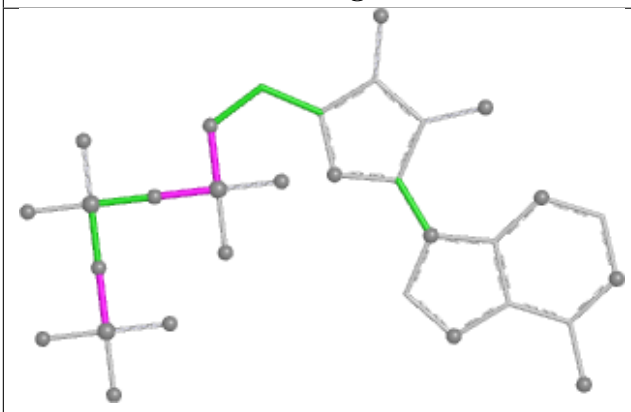
Ligand ATP D 2801



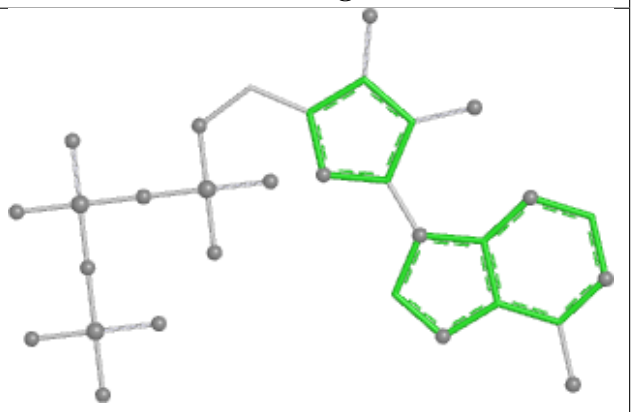
Bond lengths



Bond angles

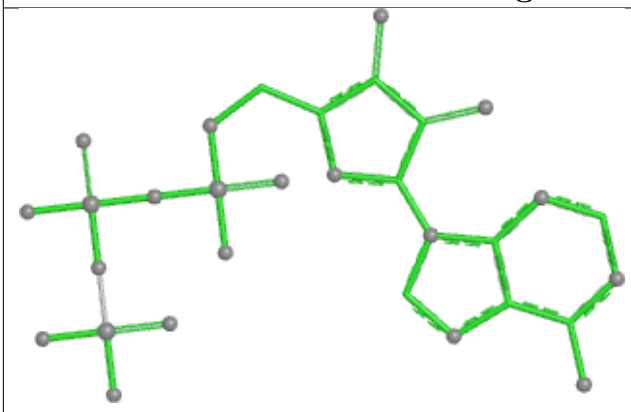


Torsions

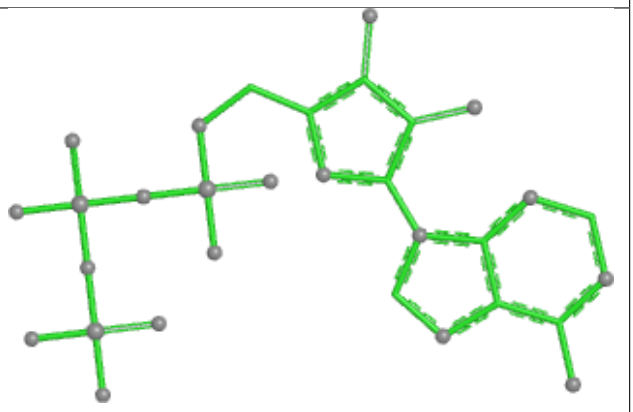


Rings

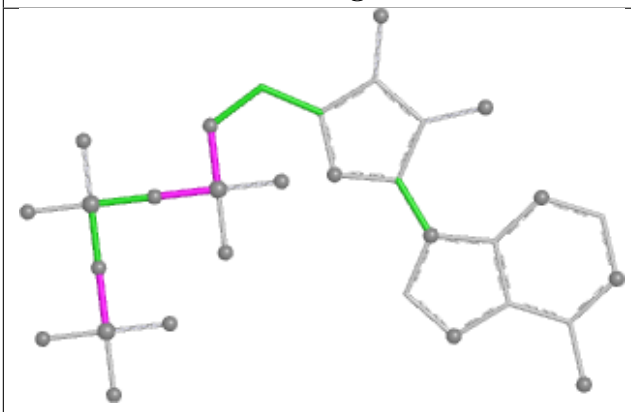
Ligand ATP C 2801



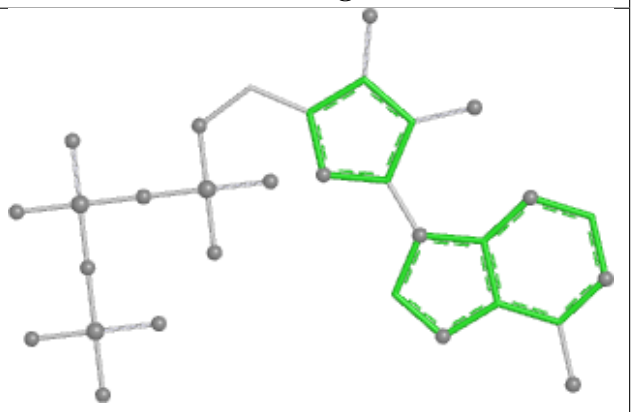
Bond lengths



Bond angles

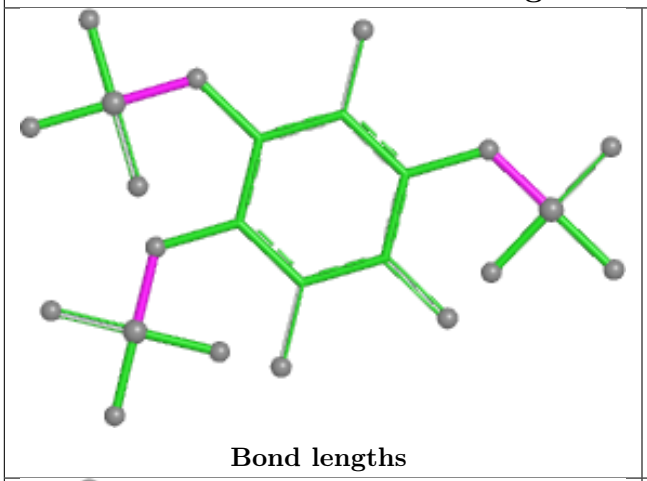


Torsions

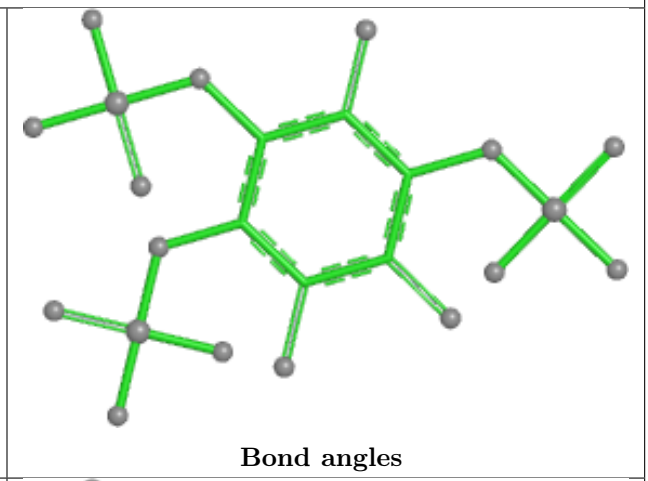


Rings

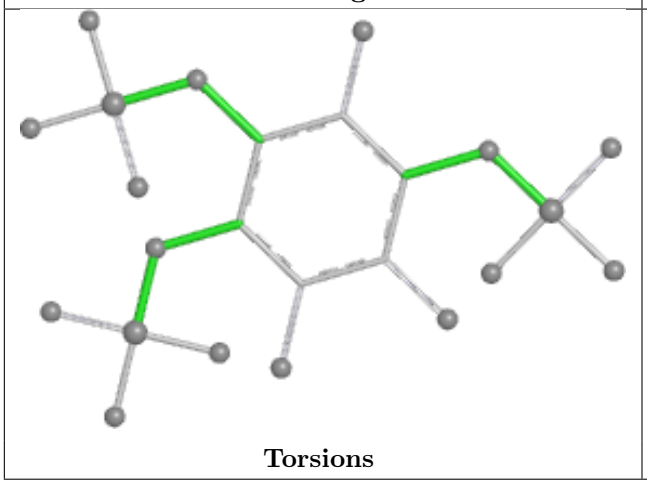
Ligand I3P A 2801



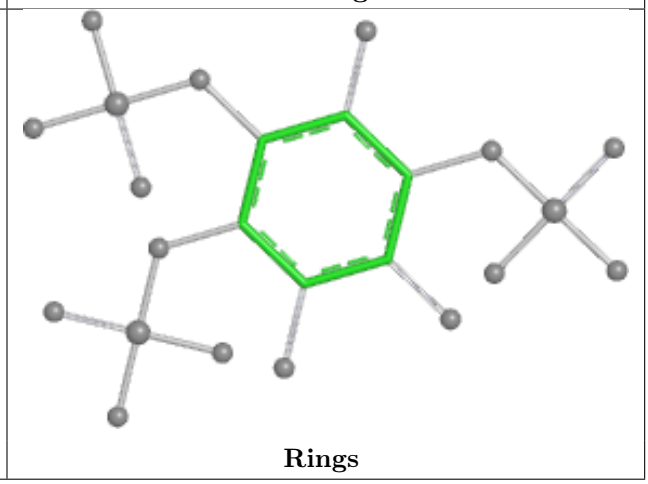
Bond lengths



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.

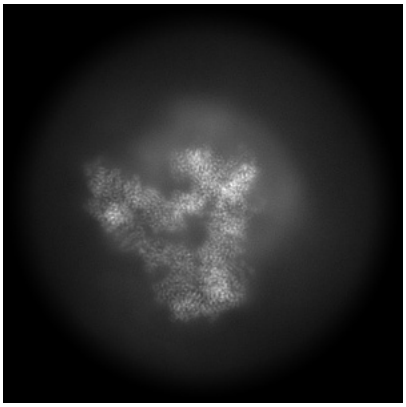
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-73129. These allow visual inspection of the internal detail of the map and identification of artifacts.

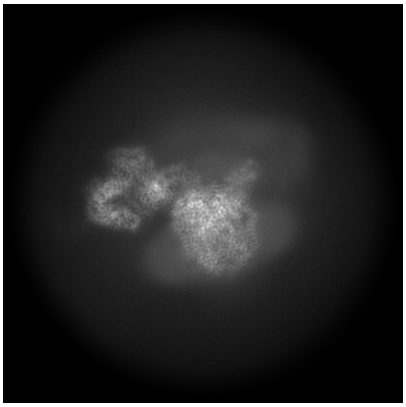
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

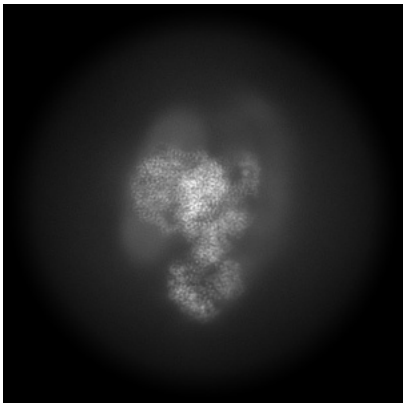
6.1.1 Primary map



X



Y

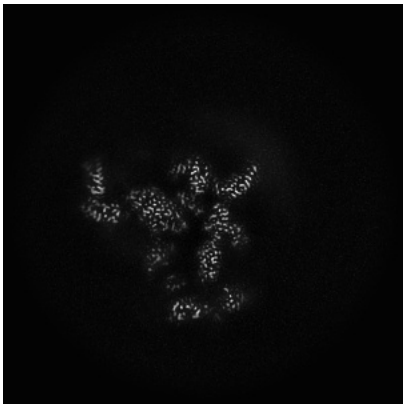


Z

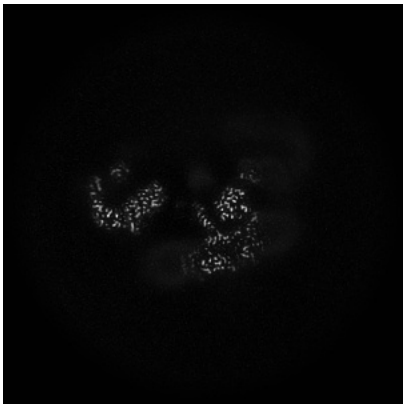
The images above show the map projected in three orthogonal directions.

6.2 Central slices

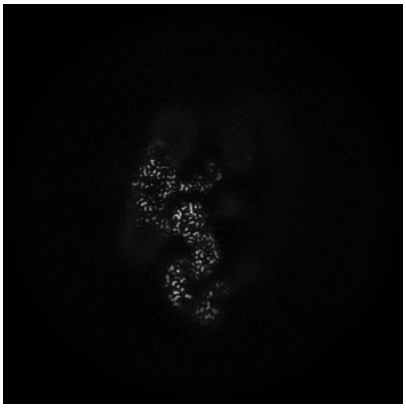
6.2.1 Primary map



X Index: 256



Y Index: 256

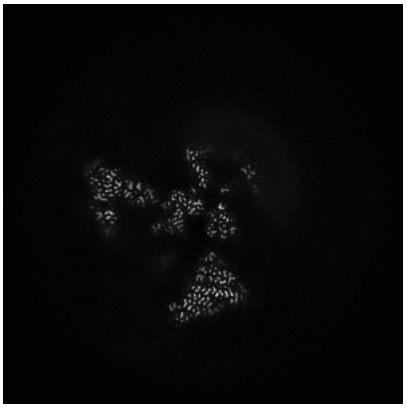


Z Index: 256

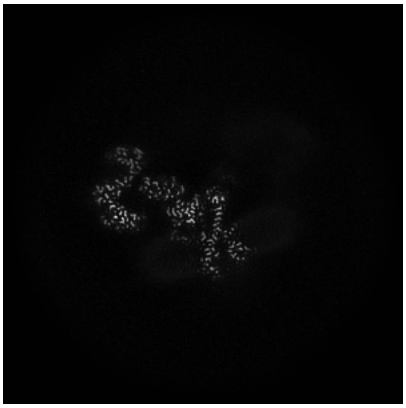
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

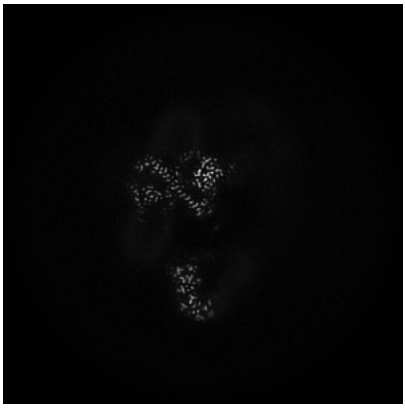
6.3.1 Primary map



X Index: 241



Y Index: 283

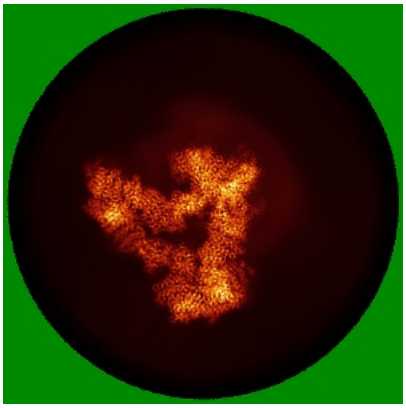


Z Index: 279

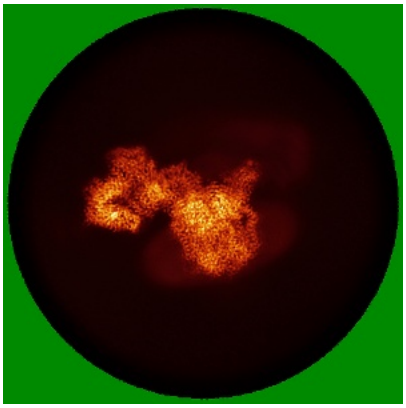
The images above show the largest variance slices of the map in three orthogonal directions.

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

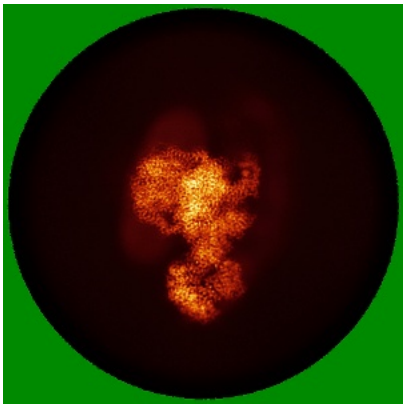
6.4.1 Primary map



X



Y

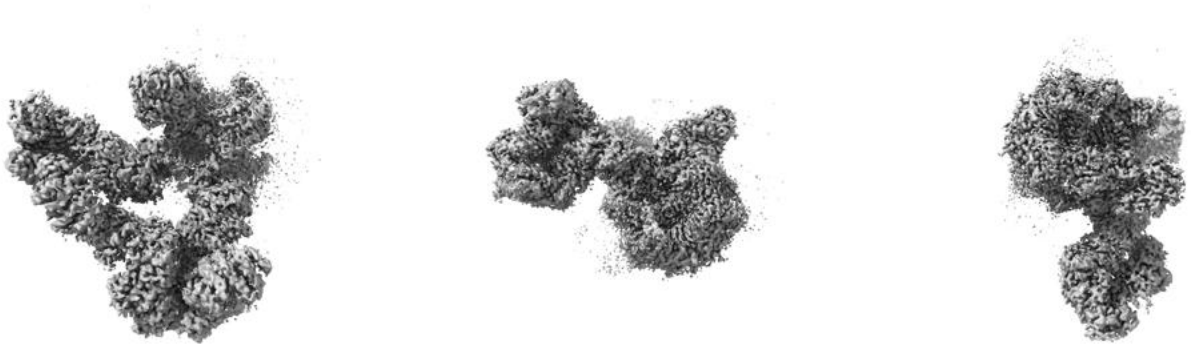


Z

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

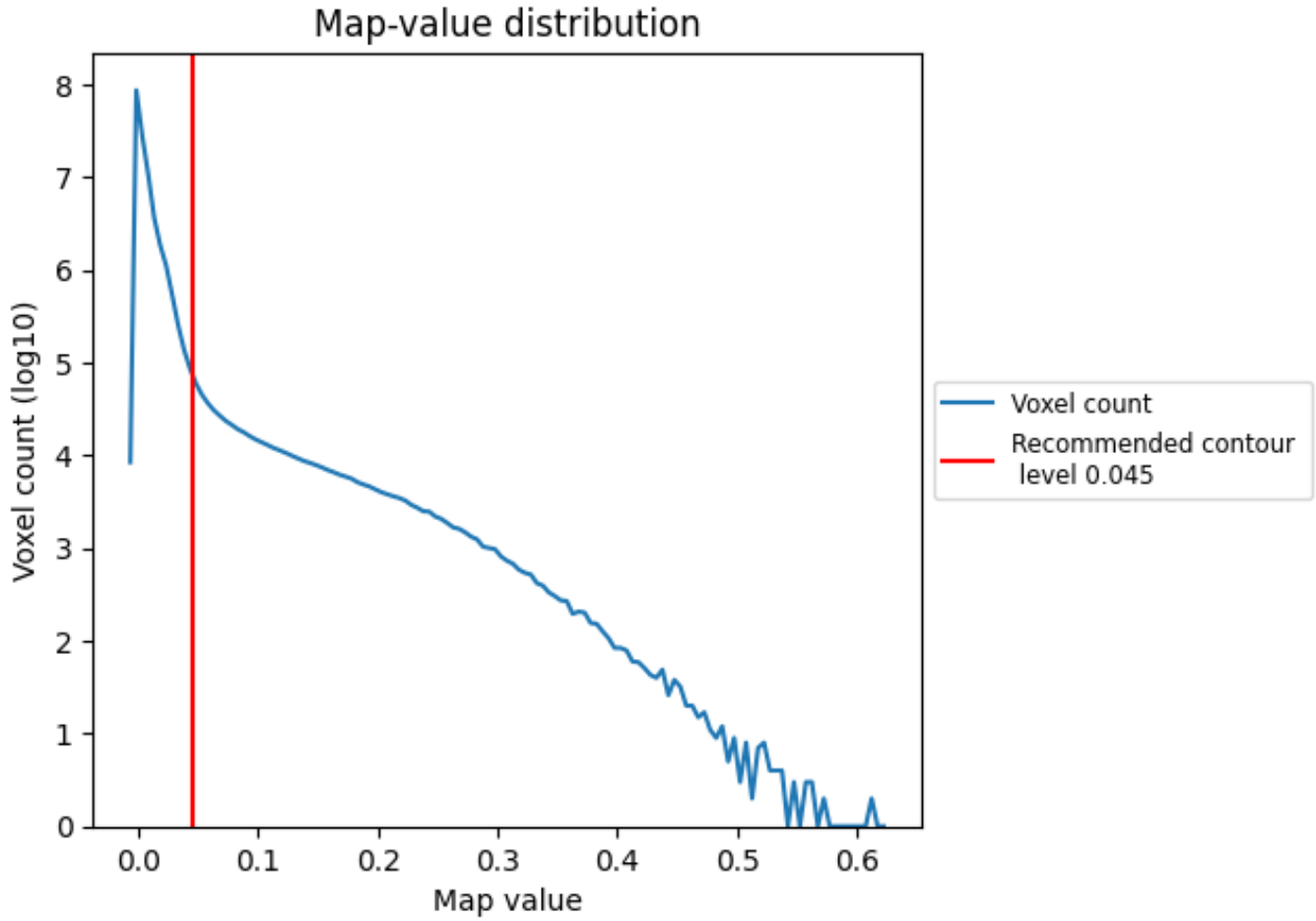
6.6 Mask visualisation (i)

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

7 Map analysis

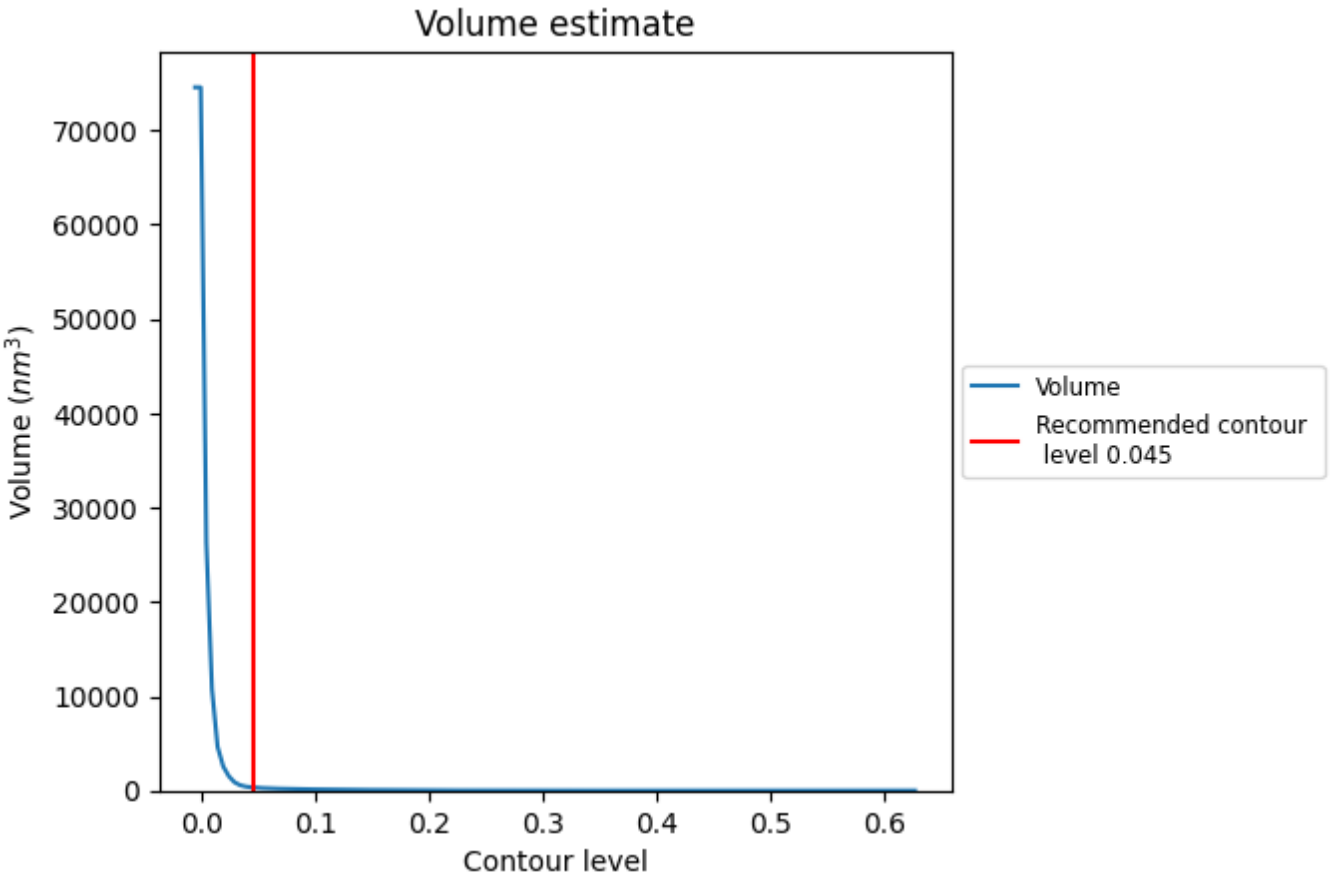
This section contains the results of statistical analysis of the map.

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.

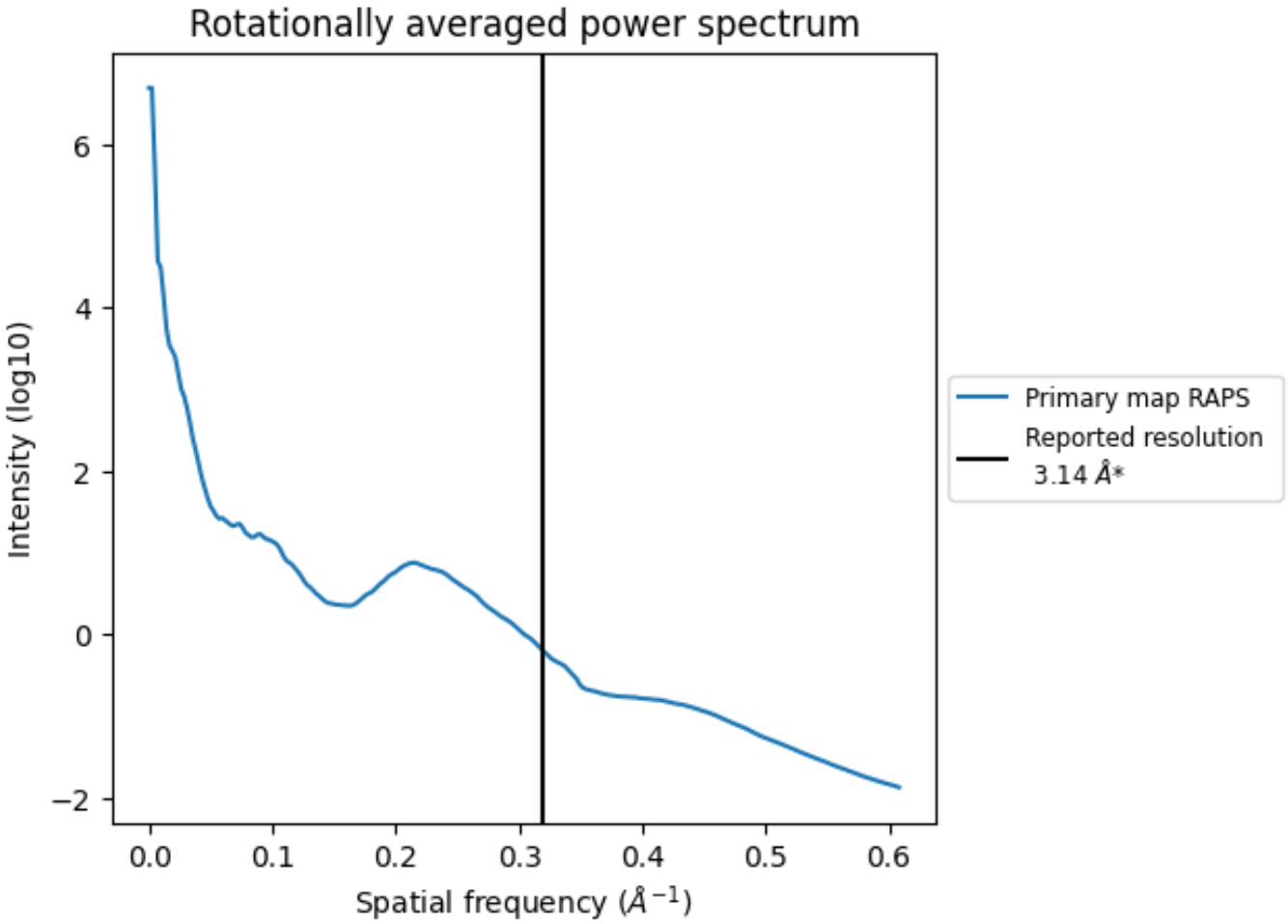
7.2 Volume estimate



The volume at the recommended contour level is 327 nm^3; this corresponds to an approximate mass of 295 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 0.318 Å^{-1}

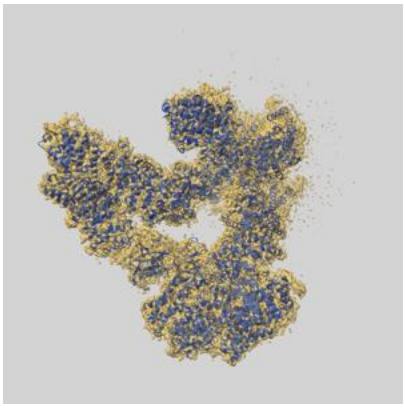
8 Fourier-Shell correlation (i)

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

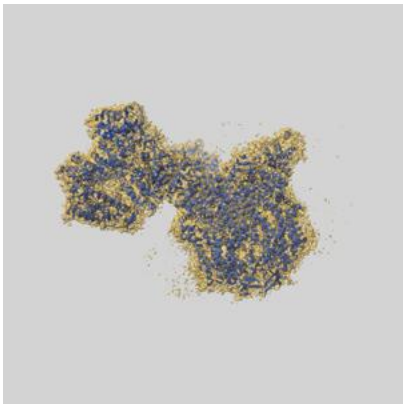
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-73129 and PDB model 9YMZ. Per-residue inclusion information can be found in section 3 on page 10.

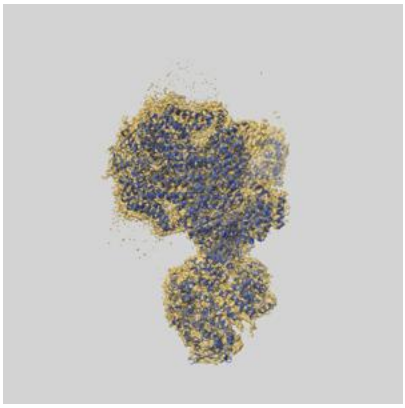
9.1 Map-model overlay



X



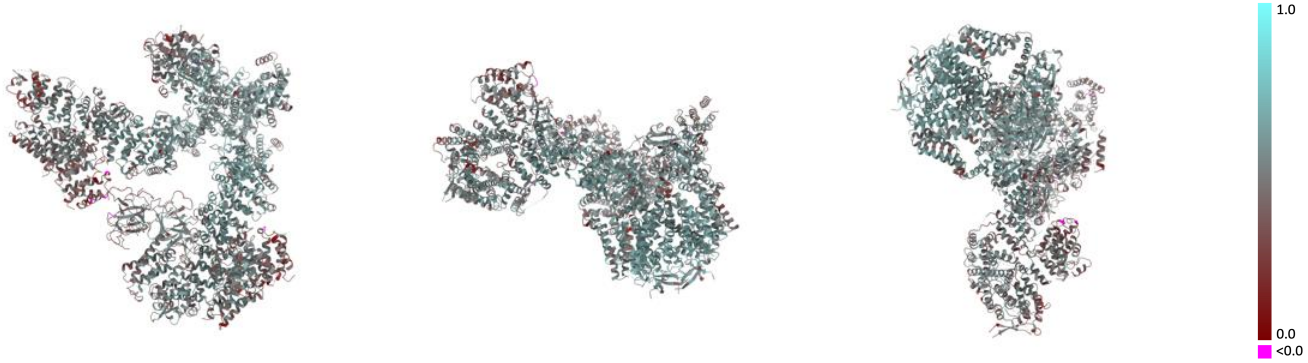
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045 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.

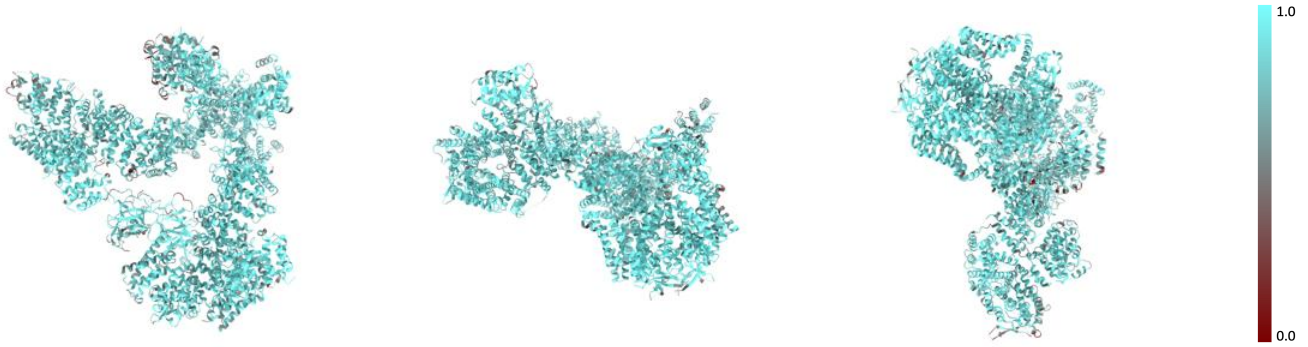
9.2 Q-score mapped to coordinate model (i)



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.

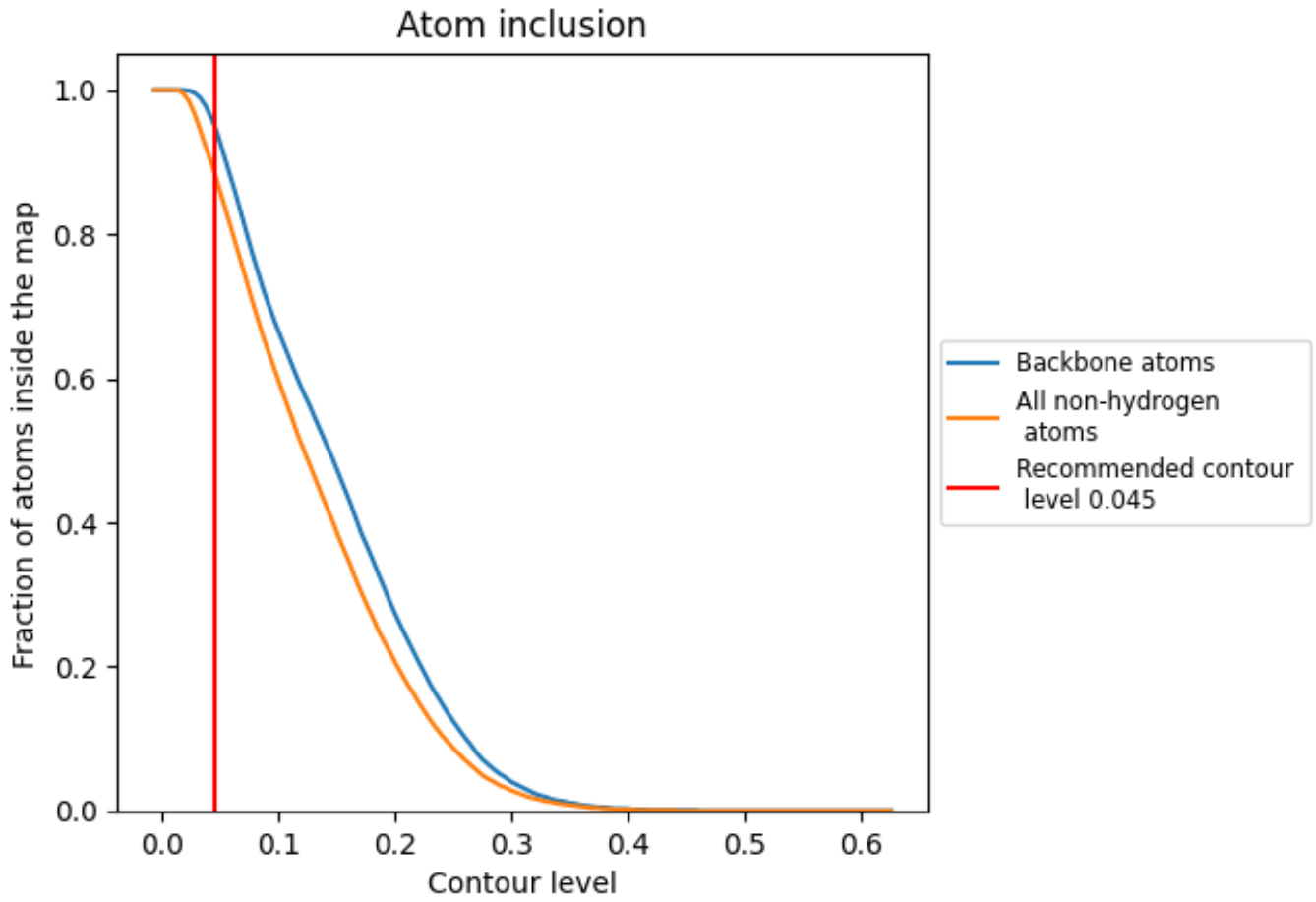
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 89% 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 (0.045) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.8880	0.5090
A	0.8920	0.5100
B	0.8850	0.4940
C	0.8560	0.5150
D	0.9190	0.5480