Full wwPDB EM Validation Report (i)

Aug 8, 2026 – 01:00 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 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 (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:

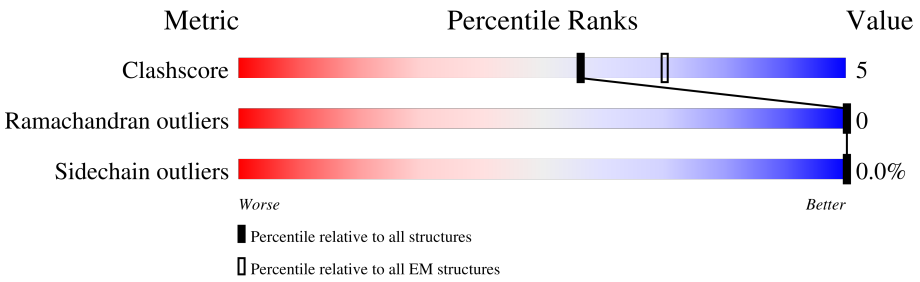
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data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

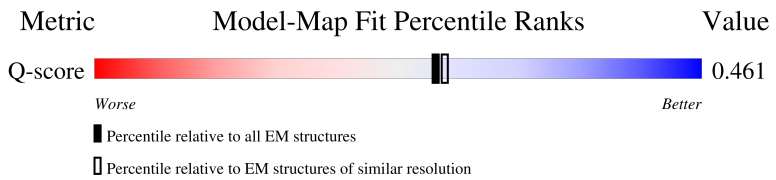
1 Overall quality at a glance (i)

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

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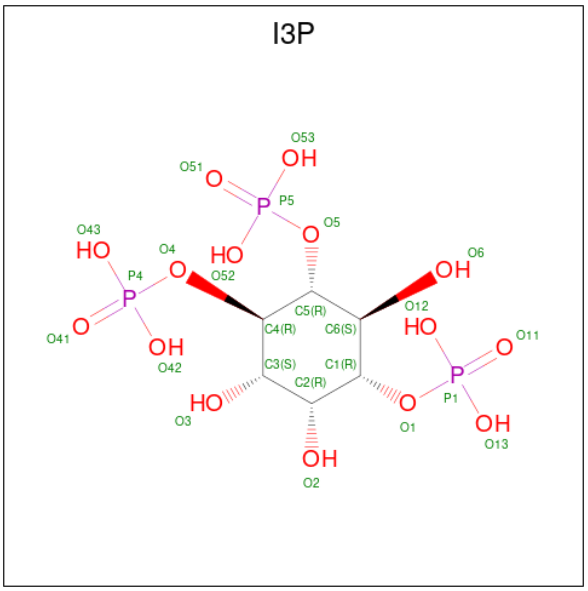
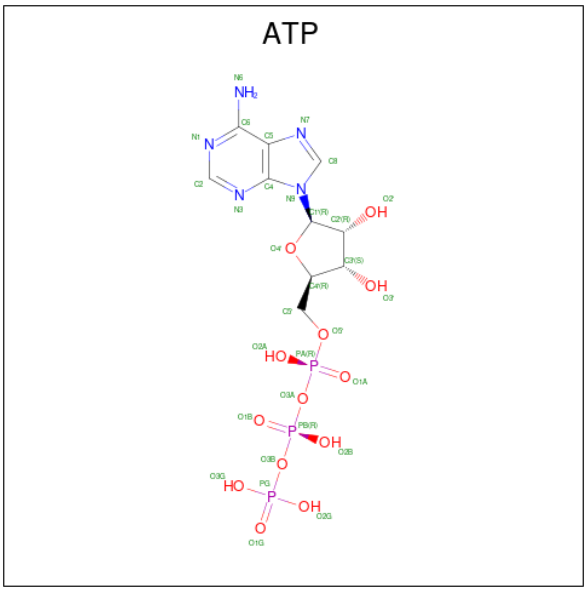
Chain	Residue	Modelled	Actual	Comment	Reference
D	2718	TRP	-	expression tag	UNP Q14571
D	2719	SER	-	expression tag	UNP Q14571
D	2720	HIS	-	expression tag	UNP Q14571
D	2721	PRO	-	expression tag	UNP Q14571
D	2722	GLN	-	expression tag	UNP Q14571
D	2723	PHE	-	expression tag	UNP Q14571
D	2724	GLU	-	expression 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
			Total	C	O	P	
2	A	1	24	6	15	3	0

- 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
			Total	C	N	O	P	
3	A	1	31	10	5	13	3	0
			Total	C	N	O	P	
3	B	1	31	10	5	13	3	0

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

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

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

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

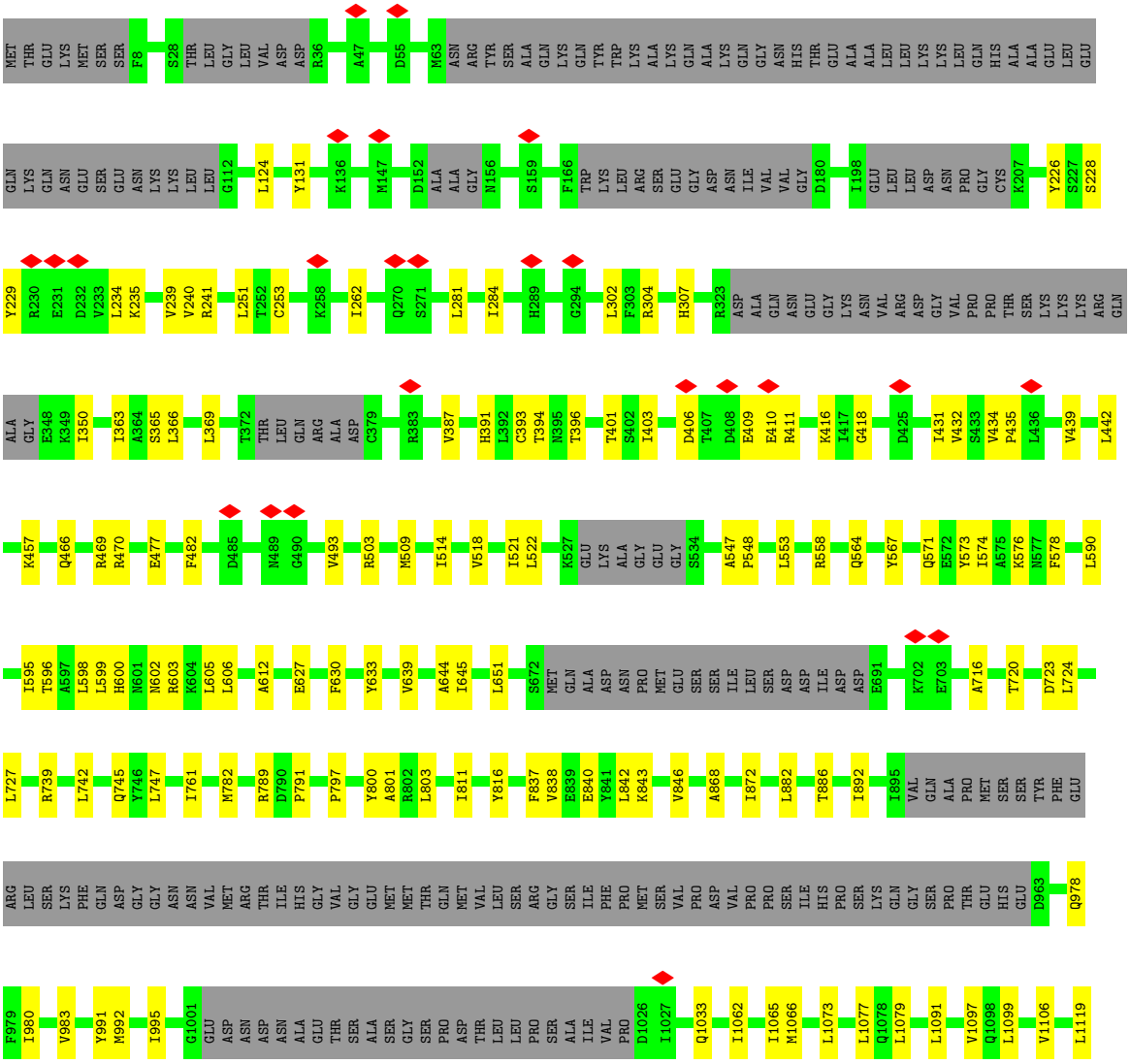
Mol	Chain	Residues	Atoms		AltConf
			Total	Ca	
5	A	1	1	1	0
5	B	1	1	1	0
5	C	1	1	1	0

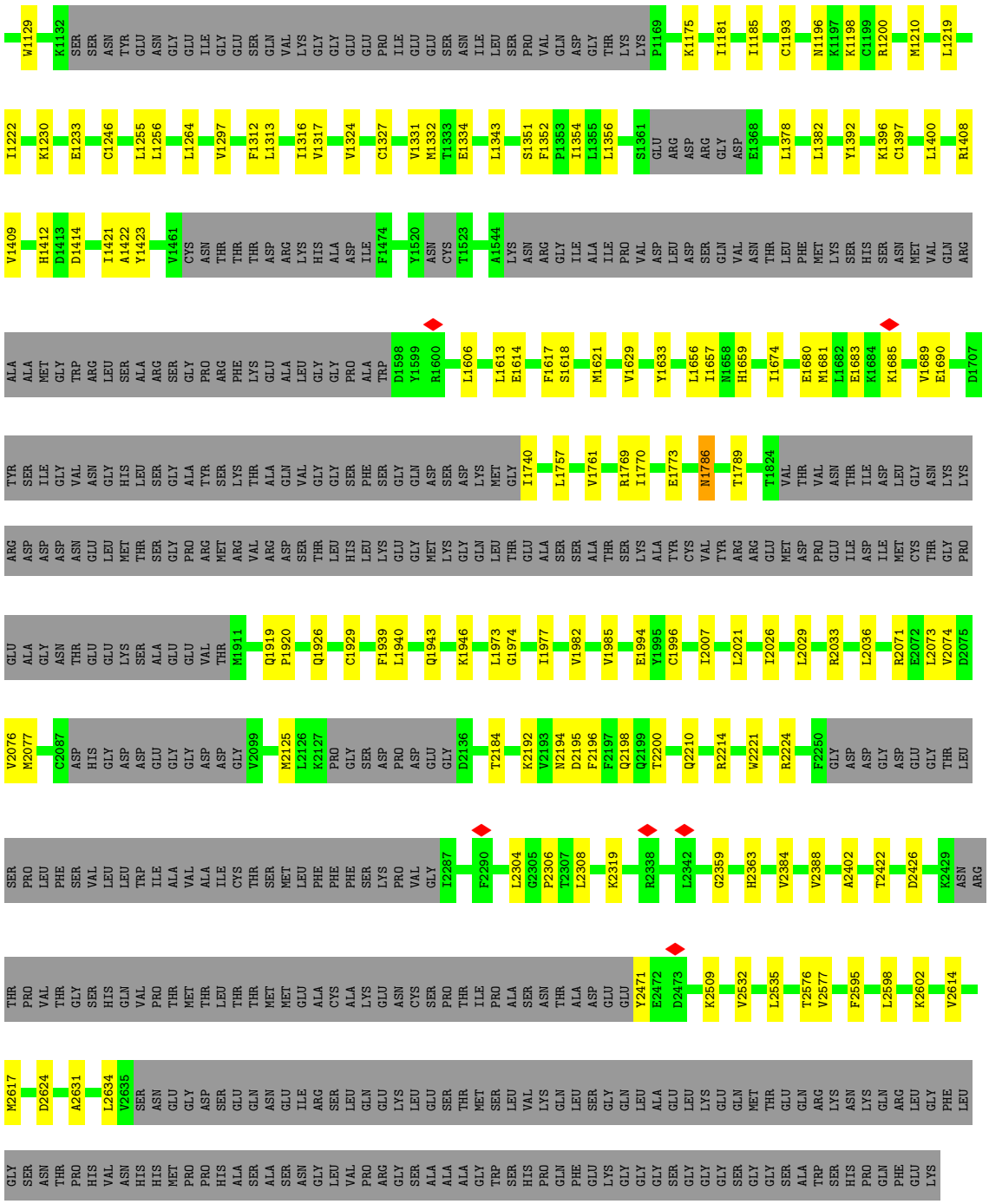
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

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

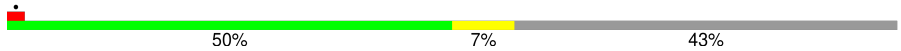
Chain A:

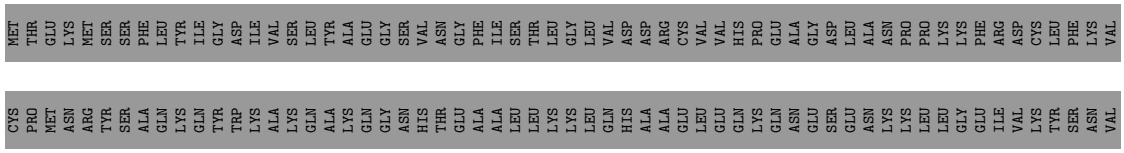


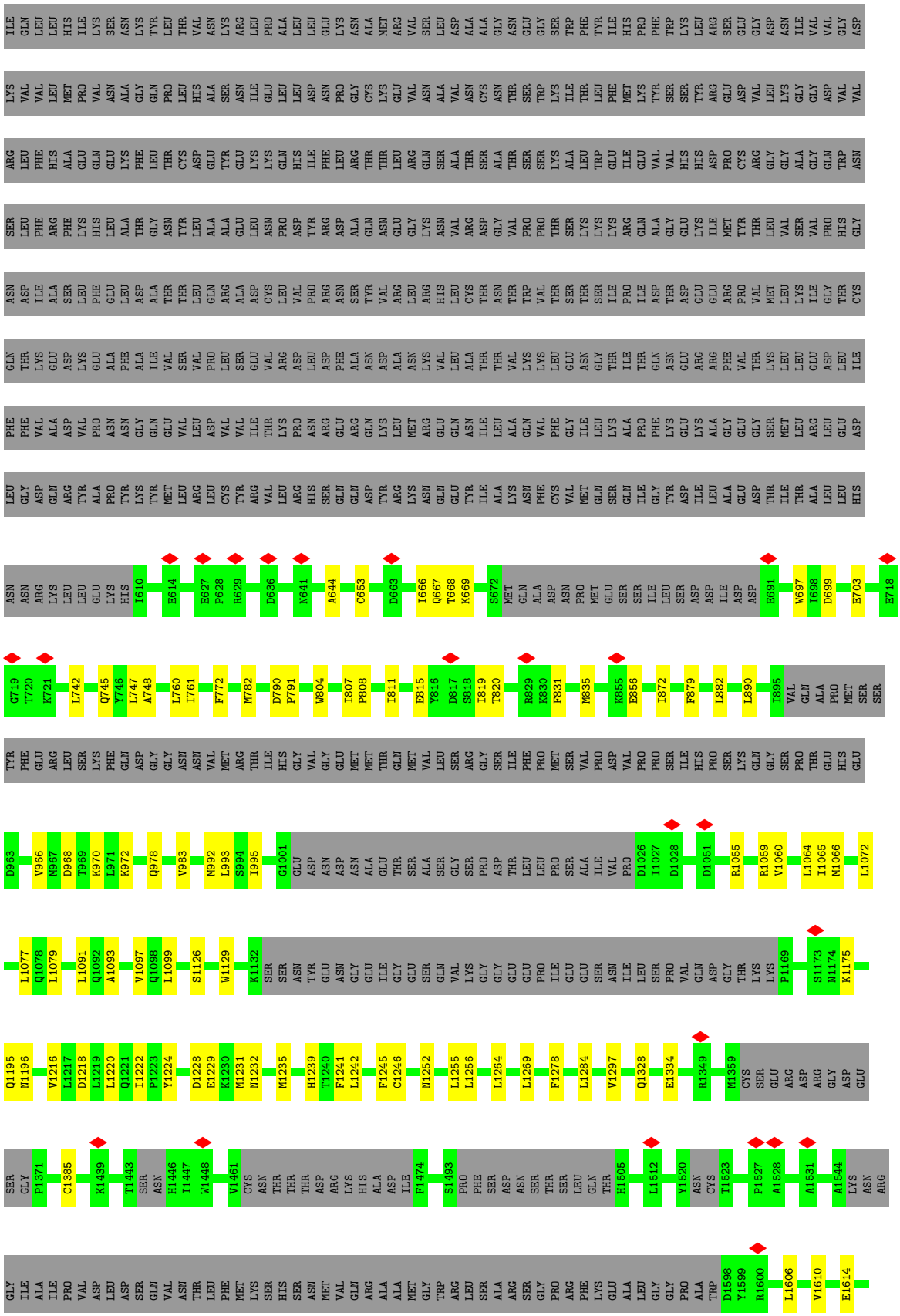


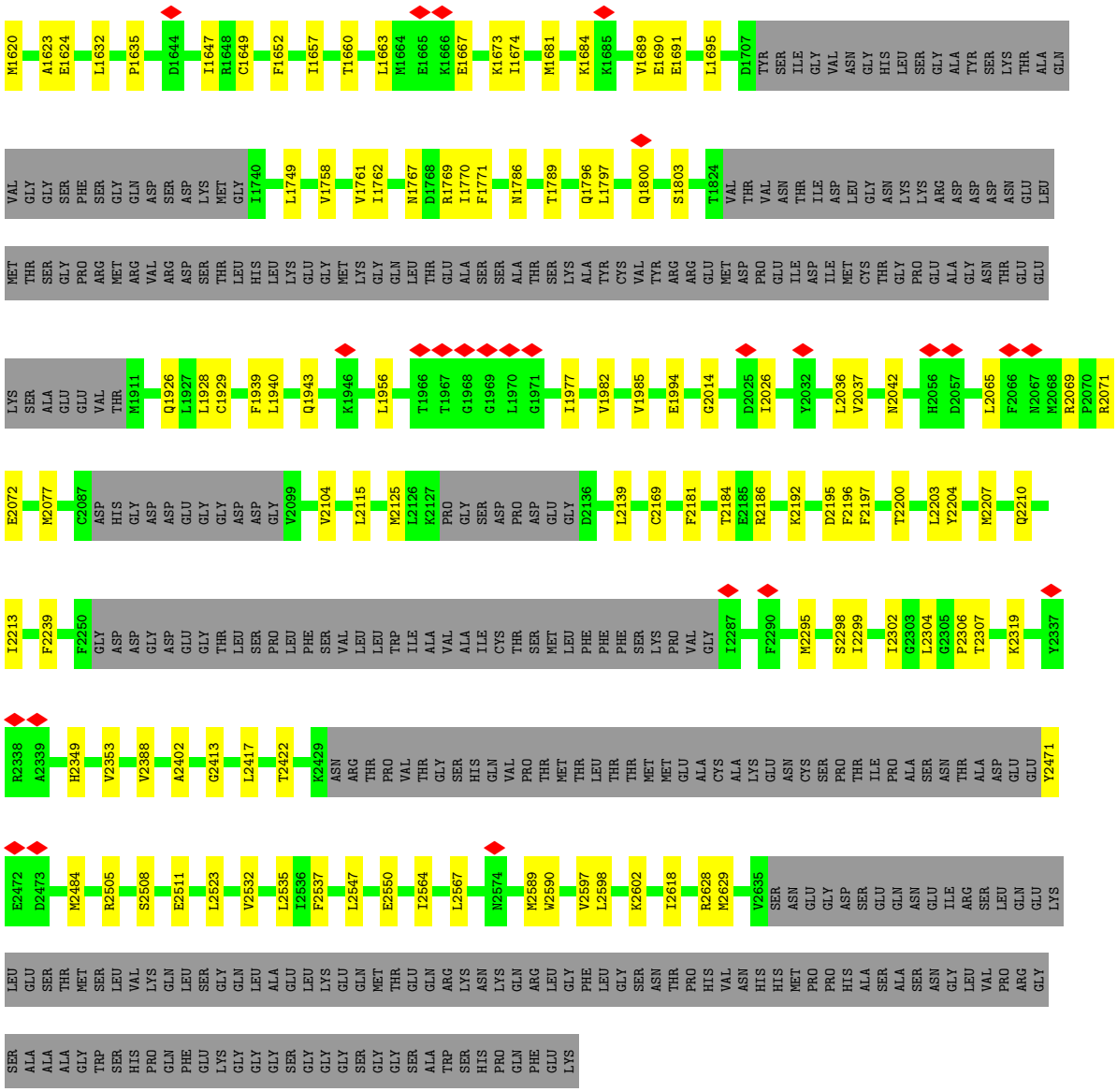
• Molecule 1: Inositol 1,4,5-trisphosphate-gated calcium channel ITPR2

Chain B:



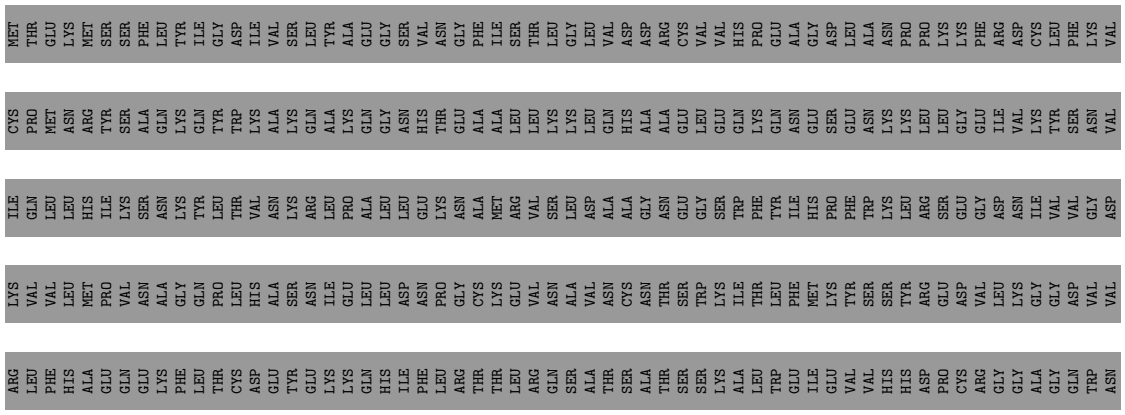


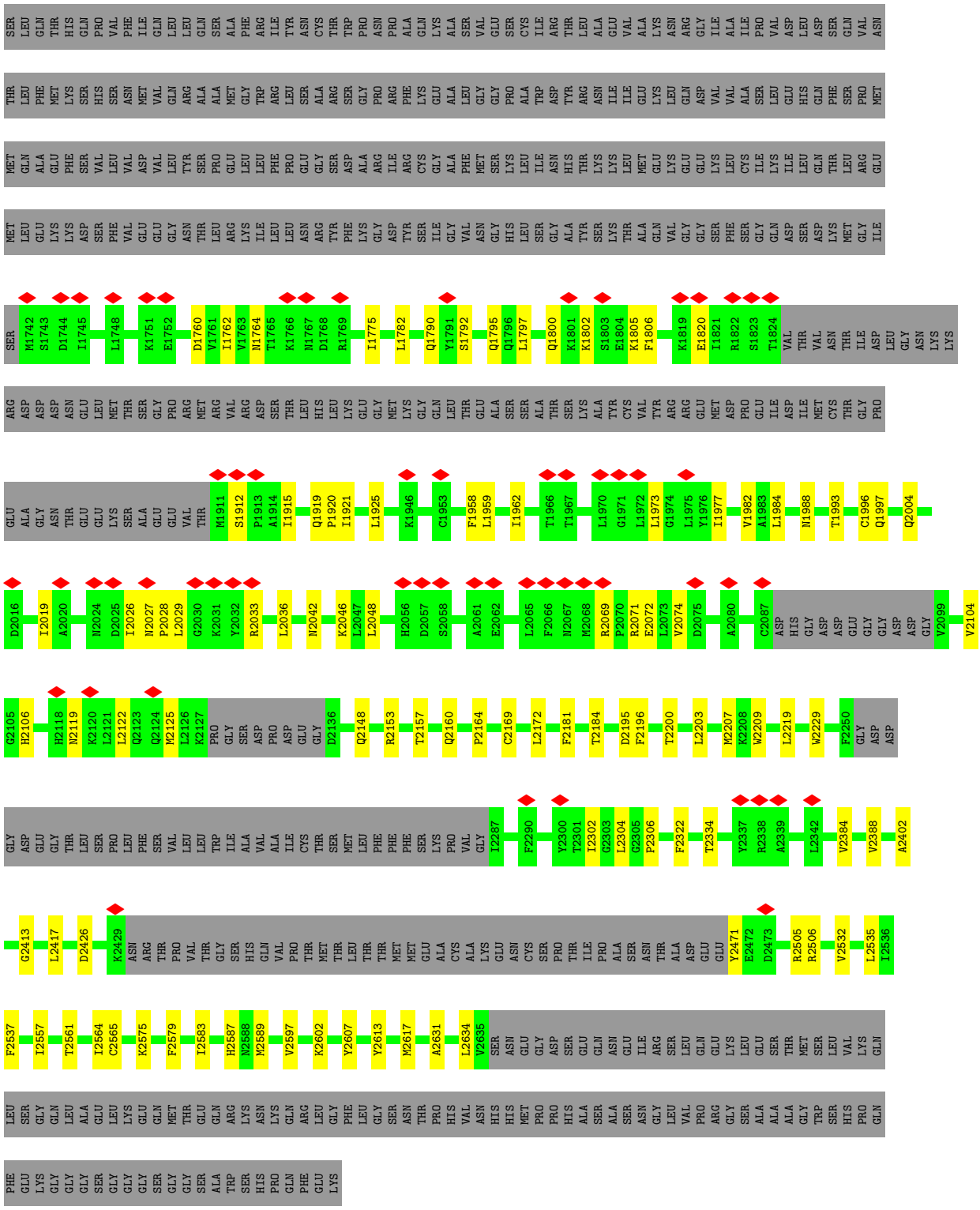

ILE GLN LEU LEU HIS ILE LYS SER ASN LYS TYR LEU THR VAL ASN LYS ARG LEU PRO ALA LEU LEU GLU LYS ASN ALA MET ARG VAL SER LEU ASP ALA GLY ASN GLU GLY SER TRP PHE TYR ILE HIS PRO PHE TRP LYS LEU ARG SER GLU GLY ASP ASN ILE VAL VAL GLY ASP
LYS VAL VAL LEU MET PRO VAL ASN ALA GLY GLN PRO LEU HIS ALA SER ASN ILE GLU LEU LEU ASP ASN PRO GLY CYS LYS GLU VAL ASN ALA VAL ASN CYS ASN THR SER TRP LYS ILE THR LEU PHE MET LYS TYR SER SER TYR ARG GLU ASP VAL LEU LYS GLY GLY ASP 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 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 ALA ALA GLU LEU ASN PRO ASP TYR ARG ASP ALA GLN ASN GLU GLY LYS ASN VAL ARG ASP GLY VAL PRO PRO THR SER LYS LYS LYS ARG GLN ALA LYS LEU MET TYR THR LEU VAL SER VAL PRO HIS GLY
ASN ASP ILE ALA SER LEU PHE GLU LEU ASP ALA 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 ASN ARG ARG ASP THR CYS
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 LYS VAL LEU ALA THR THR VAL LYS LYS LEU GLU GLN GLN THR ILE THR ILE GLN GLN GLU GLU ARG PHE VAL THR LYS LEU LEU GLU ASP LEU ILE
PHE PHE VAL ALA ASP VAL PRO ASN ASN GLY GLN GLU VAL LEU ASP VAL VAL ILE THR LYS PRO ASN ARG GLU ARG GLN LYS LEU MET ARG GLU GLN ASN ILE ILE LEU ALA GLN VAL PHE GLY ILE LEU LYS ALA PRO PHE LYS GLU LYS GLY SER MET LEU ARG LEU 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 ILE ALA LYS ASN PHE CYS VAL MET GLN SER GLN ILE GLY TYR ASP ILE ALA LEU GLU ASP THR ILE THR ALA LEU LEU HIS
ASN ASN ARG LYS LEU LEU GLU LYS HIS I610 E614 E627 P628 R629 D636 N641 A644 C653 D663 I666 Q667 T668 K669 S672 MET GLN ALA ASP ASN PRO MET GLU SER SER ILE LEU SER ASP ASP ILE ASP ASP E691 W697 I698 D699 E703 E718
G719 T720 K721 L742 Q745 Y746 L747 A748 L760 I761 F772 M782 D790 P791 W804 I807 P808 I811 E815 Y816 D817 S818 I819 T820 R829 K830 F831 M835 K855 E856 I872 F879 L882 L890 I895 VAL GLN ALA PRO MET SER SER
TYR PHE GLU ARG LEU SER LYS PHE GLN ASP GLY GLY ASN ASN VAL MET ARG THR ILE HIS GLY VAL GLY 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
D963 V966 M967 D968 T969 K970 L971 K972 Q978 V983 M992 L993 S994 I995 G1001 GLU ASP ASN ASP ASN ALA GLU THR SER ALA SER GLY SER PRO ASP THR LEU LEU PRO SER ALA ILE VAL PRO D1026 I1027 D1028 D1051 R1055 R1059 V1060 L1064 I1065 M1066 L1072
L1077 Q1078 L1079 L1091 Q1092 A1093 V1097 Q1098 L1099 S1126 W1129 K1132 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 P1169 S1173 N1174 K1175
Q1195 N1196 V1216 L1217 D1218 L1219 L1220 Q1221 I1222 P1223 Y1224 D1228 E1229 K1230 M1231 N1232 M1235 H1239 T1240 F1241 L1242 F1245 C1246 N1252 L1255 L1256 L1264 L1269 F1278 L1284 V1297 Q1328 E1334 R1349 M1359 CYS SER GLU ARG ASP ARG GLY ASP GLU
SER GLY P1371 C1385 K1439 T1443 SER ASN H1446 I1447 W1448 V1461 CYS ASN THR THR THR ASP ARG LYS HIS ALA ASP ILE F1474 S1493 PRO PHE SER ASP ASN SER THR SER LEU GLN THR H1505 L1512 Y1520 ASN CYS T1523 P1527 A1528 A1531 A1544 LYS ASN ARG
GLY ILE ALA ILE PRO VAL ASP LEU ASP SER GLN VAL ASN THR LEU PHE MET LYS SER HIS SER ASN MET VAL GLN ARG ALA ALA MET GLY TRP ARG LEU SER ALA ARG SER GLY PRO ARG PHE LYS GLU ALA LEU GLY GLY PRO ALA TRP D1598 Y1599 R1600 L1606 V1610 E1614



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

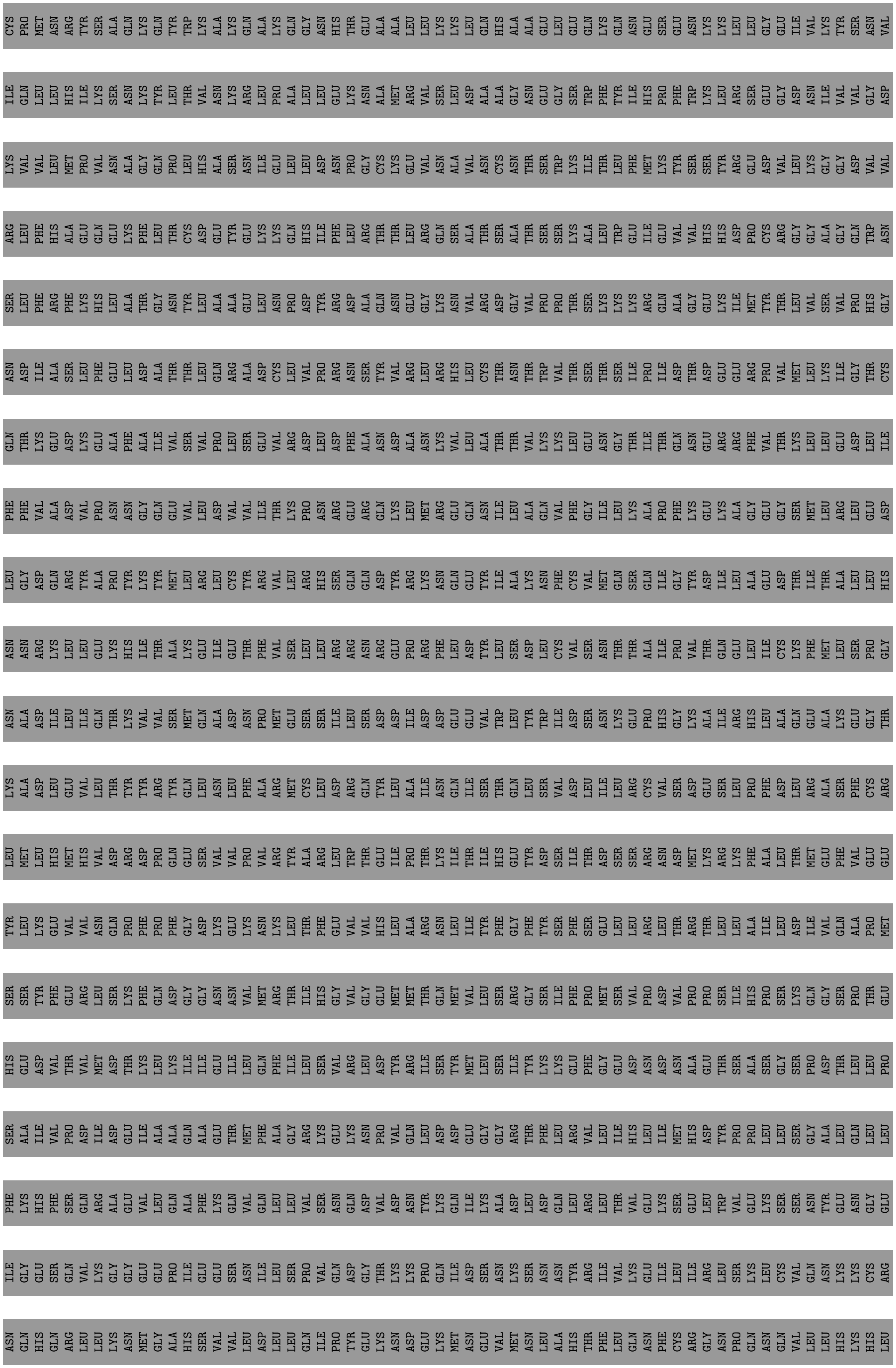
Chain C:

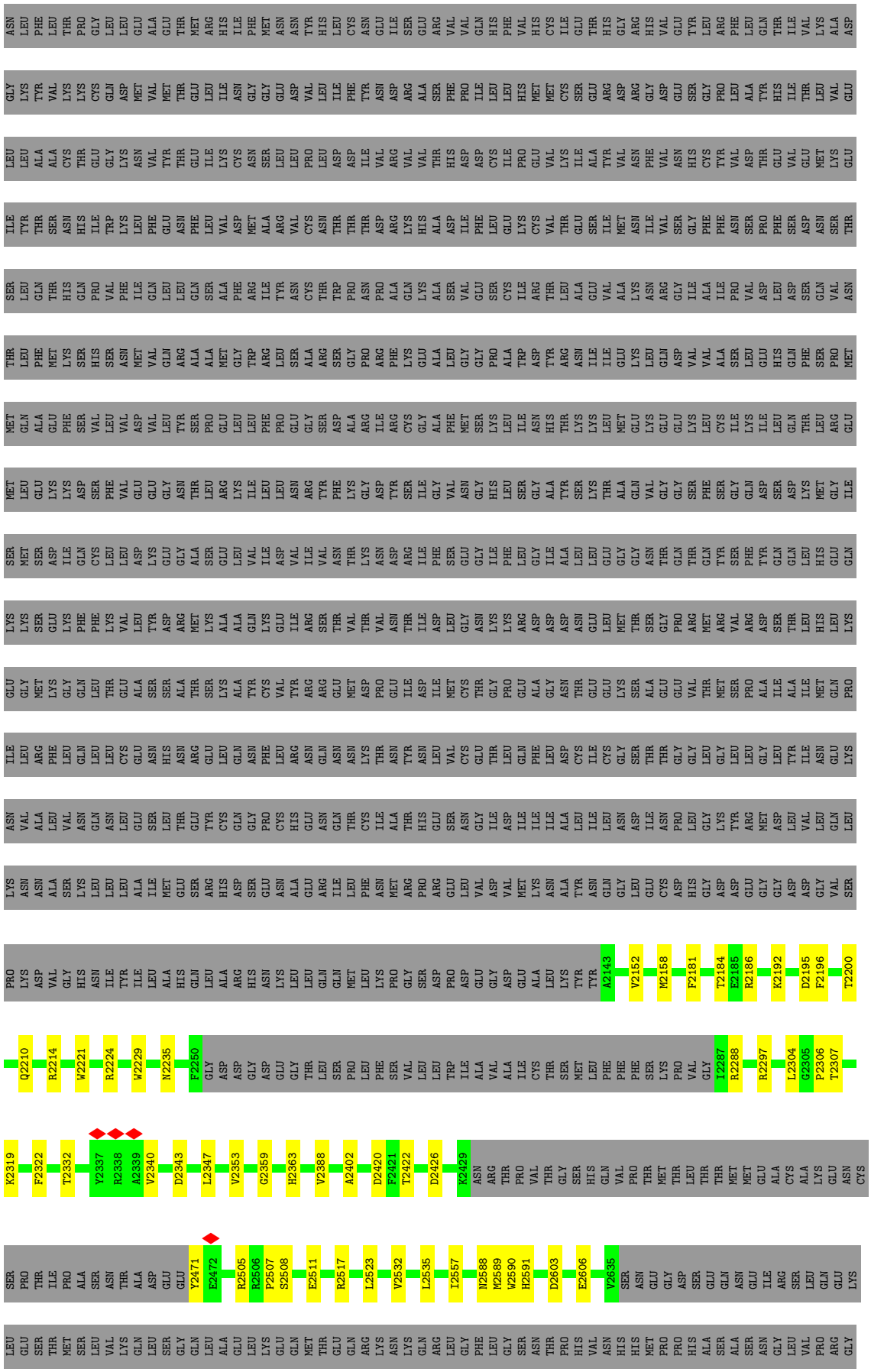




- Molecule 1: Inositol 1,4,5-trisphosphate-gated calcium channel ITPR2

Chain D: 13% • 85%




ASN LEU PHE LEU THR PRO GLY LEU LEU GLU ALA GLU THR MET ARG HIS ILE PHE MET ASN ASN TYR HIS LEU CYS ASN GLU ILE SER GLU ARG VAL VAL GLN HIS PHE VAL HIS CYS ILE GLU THR HIS GLY ARG HIS VAL GLU TYR LEU ARG PHE LEU GLN THR ILE VAL LYS ALA ASP
GLY LYS TYR VAL LYS LYS CYS GLN ASP MET VAL MET THR GLU LEU ILE ASN GLY GLU GLU ASP VAL LEU ILE PHE TYR ASN ASP ARG ALA SER PHE PRO ILE ILE LEU LEU HIS MET MET CYS SER GLU ARG ASP ARG GLY ASP GLU SER GLY PRO LEU ALA TYR HIS ILE THR LEU VAL GLU
LEU LEU ALA ALA CYS THR GLU GLY LYS ASN VAL VAL TYR THR GLU ILE LYS CYS ASN SER LEU LEU PRO LEU ASP ASP TYR VAL ARG VAL THR HIS ASP ASP CYS ILE PRO GLU VAL LYS ILE ALA TYR VAL ASN PHE VAL ASN HIS CYS TYR VAL ASP THR ASP GLU VAL GLU GLU MET LYS GLU
ILE TYR THR SER ASN HIS ILE TRP LYS LEU PHE GLU ASN PHE LEU VAL ASP MET ALA ARG VAL CYS ASN THR THR THR ASP ARG LYS HIS ALA ASP ILE PHE LEU GLU GLU SER GLU LYS CYS VAL THR GLU SER ILE MET ASN ILE VAL SER GLY PHE PHE ASN SER PRO PHE SER ASP ASN THR
SER LEU GLN THR HIS GLN PRO VAL PHE ILE GLN LEU GLN SER ALA ALA PHE ARG ILE TYR ASN CYS THR TRP PRO ASN PRO ALA GLN LYS ALA SER VAL GLU SER CYS ILE ILE ARG THR LEU ALA GLU VAL ALA LYS ASN GLY ILE ALA ILE PRO VAL ASP LEU ASP SER GLN GLN ASN VAL
THR LEU PHE MET LYS SER HIS SER ASN MET VAL GLN ARG ALA ALA MET GLY TRP ARG LEU SER ALA ARG SER GLY PRO ARG PHE ALA LEU GLY GLY PRO ALA TRP ASP TYR ARG LEU GLU GLU LYS LEU GLU HIS GLN PHE SER PRO MET
MET GLN ALA GLU PHE SER VAL LEU VAL ASP VAL LEU TYR SER PRO GLU LEU LEU PHE PRO GLU GLY SER ASP ALA ARG ILE ARG CYS GLY ALA PHE MET SER LYS LEU ILE ILE ASN HIS THR LYS LYS LEU MET GLU LYS GLU GLU LYS LYS CYS ILE LYS LEU LEU ARG GLU
MET LEU GLU LYS LYS ASP SER PHE VAL GLU GLU GLY ASN THR LEU ARG LYS ILE LEU LEU ASN ARG TYR PHE LYS GLY ASP TYR SER ILE GLY VAL ASN GLY HIS LEU SER GLY ALA TYR SER LYS THR ALA GLN VAL GLY GLY SER PHE SER GLY GLN ASP VAL LYS LEU CYS ILE LYS LYS ILE
SER MET SER ASP ILE GLN CYS LEU LEU ASP LYS GLU GLY ALA SER GLU LEU VAL ILE ASP VAL ILE VAL ASN THR LYS ASN ASP ARG ILE PHE SER GLU GLY ILE ALA LEU LEU GLU GLN THR GLN TYR SER PHE TYR GLN LEU GLN GLN
LYS LYS SER GLU LYS PHE PHE LYS VAL LEU TYR ASP ARG MET LYS ALA ALA GLN LYS GLU VAL THR VAL ASN THR ILE ASP LEU GLY ASN LYS LYS ARG ASP ASP ASN GLU LEU MET THR SER GLY PRO ARG MET ARG VAL ARG ASP SER THR LEU HIS LEU LYS
GLU GLY MET LYS GLY GLN LEU THR GLU ALA SER SER ALA THR SER LYS ALA TYR CYS VAL TYR ARG ARG GLU MET ASP PRO GLU ILE ASP ILE MET CYS THR GLY PRO GLU ALA GLY ASN THR GLU GLU LYS SER ALA GLU GLU VAL THR ARG GLU GLU PRO ALA ILE ALA ILE MET GLN PRO
ILE LEU ARG PHE LEU GLN LEU LEU CYS GLU ASN HIS ASN ARG GLU LEU GLN ASN PHE LEU ARG ASN GLN ASN ASN LYS THR ASN TYR ASN LEU VAL CYS GLU TRP LEU LEU GLY GLY GLY SER THR THR GLY GLY LEU GLY LEU LEU GLY LEU GLY LYS LYS
ASN VAL ALA LEU VAL ASN GLN ASN LEU GLU SER LEU THR GLU TYR CYS GLN GLY PRO CYS HIS GLU ASN GLN THR CYS ILE ALA THR HIS GLU SER GLU GLY ILE ALA LEU ILE LEU ASP ILE ILE ILE ALA LEU ILE LEU ASP ASN PRO LEU GLY LYS TYR ARG MET ASP LEU GLN GLU
LYS ASN ASN ALA SER LYS LEU LEU LEU ALA ILE MET GLU SER ARG HIS ASP SER GLU ASN ALA GLU ARG ILE LEU PHE ASN MET ARG PRO ARG GLU GLU LEU VAL ASP VAL MET LYS ASN ALA TYR ASN GLN GLY LEU GLU CYS ASP HIS GLY ASP ASP GLU GLY GLY GLY ASP LEU LEU SER
PRO LYS ASP VAL GLY HIS ASN ILE TYR ILE LEU ALA HIS GLN LEU ALA ARG HIS ASN LYS LEU LEU MET LEU LYS PRO LEU GLN GLN MET LEU LYS TYR TYR A2143 V2152 M2158 F2181 T2184 E2185 R2186 K2192 D2195 F2196 T2200
Q2210 R2214 W2221 R2224 W2229 N2235 F2250 GLY ASP ASP GLY ASP GLU GLY THR LEU SER PRO LEU PHE SER VAL LEU LEU TRP ILE ALA VAL ALA ILE CYS THR SER MET LEU PHE PHE PHE SER LYS PRO VAL GLY 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 ASN ARG THR PRO VAL THR GLY SER HIS GLN VAL PRO THR MET THR LEU THR THR MET MET GLU ALA CYS ALA LYS GLU ASN CYS
SER PRO THR ILE PRO ALA SER ASN THR ALA ASP GLU GLU Y2471 E2472 R2505 R2506 P2507 S2508 E2511 R2517 L2523 V2532 L2535 I2557 N2588 M2589 W2590 H2591 D2603 E2606 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 ARG LEU GLY PHE LEU GLY GLN 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
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	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 (i)

5.1 Standard geometry (i)

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	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

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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
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.

All (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
1:B:1926:GLN:HG3	1:B:1994:GLU:HG3	1.74	0.70
1:A:564:GLN:HB3	1:A:574:ILE:HD12	1.73	0.69
1:A:477:GLU:HG3	1:A:493:VAL:HG11	1.73	0.69
1:A:846:VAL:HG12	1:A:892:ILE:HG13	1.75	0.69
1:A:761:ILE:HG21	1:A:782:MET:HB2	1.76	0.68
1:C:1760:ASP:O	1:C:1764:ASN:HB2	1.93	0.68
1:C:1958:PHE:HE2	1:C:1984:LEU:HD21	1.59	0.68
1:C:2402:ALA:HB2	1:C:2532:VAL:HG11	1.76	0.67
1:D:2402:ALA:HB2	1:D:2532:VAL:HG11	1.74	0.67
1:C:1762:ILE:HD12	1:C:1775:ILE:HD11	1.78	0.66
1:A:241:ARG:HB2	1:A:432:VAL:HB	1.77	0.65
1:B:761:ILE:HG21	1:B:782:MET:HB2	1.78	0.65
1:A:995:ILE:HG12	1:A:1033:GLN:HG2	1.78	0.64
1:B:790:ASP:HB3	1:B:791:PRO:HD3	1.79	0.64
1:B:1956:LEU:HD11	1:B:2014:GLY:HA3	1.79	0.64
1:C:1762:ILE:HD13	1:C:1806:PHE:HE1	1.63	0.64
1:A:1077:LEU:HD13	1:A:1674:ILE:HD11	1.80	0.63
1:A:234:LEU:HD11	1:A:284:ILE:HG13	1.80	0.62
1:A:596:THR:O	1:A:600:HIS:HB2	1.99	0.62
1:A:1332:MET:HE1	1:A:1382:LEU:HD22	1.80	0.62
1:C:2631:ALA:HB3	1:C:2634:LEU:HD23	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:VAL:HG23	1:A:434:VAL:HB	1.81	0.62
1:A:1629:VAL:HG13	1:A:1681:MET:HG2	1.81	0.61
1:B:1099:LEU:HD22	1:B:1606:LEU:HD22	1.83	0.61
1:C:2029:LEU:HD11	1:C:2036:LEU:HD22	1.82	0.61
1:A:2033:ARG:HE	1:A:2036:LEU:HD11	1.66	0.60
1:A:1129:TRP:HA	1:A:1175:LYS:HD3	1.82	0.60
1:C:2019:ILE:HG22	1:C:2048:LEU:HD11	1.83	0.60
1:A:1973:LEU:HD21	1:A:2021:LEU:HD23	1.82	0.60
1:C:2304:LEU:O	1:C:2306:PRO:HD2	2.02	0.60
1:A:2471:TYR:HE2	1:D:2422:THR:HG21	1.67	0.59
1:A:789:ARG:HG3	1:A:791:PRO:HD2	1.85	0.58
1:A:1629:VAL:HG21	1:A:1680:GLU:HG3	1.84	0.58
1:D:2152:VAL:HG22	1:D:2158:MET:HG2	1.85	0.58
1:C:2565:CYS:SG	1:C:2587:HIS:CE1	2.96	0.58
1:A:1657:ILE:HG23	1:A:1757:LEU:HD22	1.86	0.57
1:B:2186:ARG:HB3	1:B:2192:LYS:HG2	1.86	0.57
1:C:2184:THR:HG23	1:C:2195:ASP:HB3	1.85	0.57
1:A:1062:ILE:HG22	1:A:1066:MET:HE2	1.87	0.57
1:C:2535:LEU:HD21	1:D:2388:VAL:HG23	1.87	0.57
1:A:2598:LEU:O	1:A:2602:LYS:HB2	2.04	0.56
1:D:2304:LEU:O	1:D:2306:PRO:HD2	2.05	0.56
1:A:2304:LEU:O	1:A:2306:PRO:HD2	2.06	0.56
1:B:2304:LEU:O	1:B:2306:PRO:HD2	2.06	0.56
1:B:2535:LEU:HD21	1:C:2388:VAL:HG23	1.88	0.56
1:B:1242:LEU:HD22	1:B:1256:LEU:HD11	1.88	0.56
1:A:801:ALA:HB3	1:A:1210:MET:HE3	1.88	0.55
1:C:2564:ILE:HD11	1:C:2589:MET:HB3	1.89	0.55
1:B:808:PRO:HD2	1:B:811:ILE:HD11	1.87	0.55
1:B:1229:GLU:HA	1:B:1232:ASN:HB2	1.87	0.55
1:A:350:ILE:HD11	1:A:416:LYS:HE2	1.89	0.55
1:A:469:ARG:HD3	1:A:548:PRO:HB2	1.90	0.54
1:D:2186:ARG:HH11	1:D:2557:ILE:HD13	1.72	0.54
1:D:2184:THR:HG23	1:D:2195:ASP:HB3	1.88	0.54
1:C:1993:THR:O	1:C:1997:GLN:HG3	2.06	0.54
1:A:2071:ARG:HH21	1:A:2125:MET:HE2	1.72	0.54
1:B:699:ASP:HB2	1:B:703:GLU:HB2	1.89	0.54
1:C:2169:CYS:HA	1:C:2207:MET:HE3	1.88	0.54
1:C:2302:ILE:HD12	1:C:2306:PRO:HB2	1.90	0.54
1:A:1982:VAL:HG21	1:A:2036:LEU:HB3	1.89	0.54
1:B:2197:PHE:HZ	1:B:2618:ILE:HG23	1.73	0.54
1:A:522:LEU:HD23	1:A:553:LEU:HD22	1.88	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2388:VAL:HG23	1:D:2535:LEU:HD21	1.90	0.53
1:A:2033:ARG:HH21	1:A:2036:LEU:HD21	1.73	0.53
1:B:1632:LEU:HD13	1:B:1652:PHE:HE2	1.73	0.53
1:A:124:LEU:HA	1:A:131:TYR:HA	1.90	0.53
1:A:2535:LEU:HD21	1:B:2388:VAL:HG23	1.91	0.53
1:B:1091:LEU:HD21	1:B:1614:GLU:HG2	1.90	0.53
1:A:1939:PHE:O	1:A:1943:GLN:HG3	2.08	0.53
1:A:811:ILE:HG21	1:A:991:TYR:HA	1.89	0.53
1:B:1328:GLN:HG2	1:B:1385:CYS:HA	1.90	0.53
1:A:639:VAL:HB	1:A:739:ARG:HH11	1.74	0.53
1:D:2508:SER:HB3	1:D:2511:GLU:HG3	1.90	0.53
1:A:558:ARG:HH21	1:A:590:LEU:HD13	1.72	0.53
1:A:720:THR:HG22	1:A:723:ASP:H	1.74	0.53
1:D:2186:ARG:NH1	1:D:2557:ILE:HD13	2.24	0.53
1:B:644:ALA:HB2	1:B:742:LEU:HD23	1.92	0.52
1:A:251:LEU:HG	1:A:262:ILE:HD11	1.90	0.52
1:A:978:GLN:HG2	1:A:1079:LEU:HD21	1.91	0.52
1:B:2169:CYS:HA	1:B:2207:MET:SD	2.50	0.52
1:C:2042:ASN:HB2	1:C:2104:VAL:HG22	1.90	0.52
1:B:667:GLN:HB3	1:B:669:LYS:HE3	1.91	0.52
1:B:2505:ARG:HG3	1:C:2426:ASP:HB2	1.90	0.52
1:C:1993:THR:HG22	1:C:1997:GLN:HE21	1.74	0.51
1:C:2074:VAL:HG21	1:C:2125:MET:SD	2.51	0.51
1:A:281:LEU:HD12	1:A:442:LEU:HD13	1.92	0.51
1:D:2181:PHE:HB2	1:D:2589:MET:HE1	1.92	0.51
1:B:831:PHE:O	1:B:835:MET:HE3	2.11	0.51
1:A:1977:ILE:HD12	1:A:1985:VAL:HG21	1.93	0.51
1:A:363:ILE:HD12	1:A:366:LEU:HD12	1.92	0.51
1:A:603:ARG:HG3	1:A:645:ILE:HD11	1.92	0.51
1:A:391:HIS:CE1	1:A:393:CYS:HB3	2.46	0.50
1:B:1297:VAL:HG21	1:B:1334:GLU:HB3	1.93	0.50
1:B:1064:LEU:HG	1:B:1072:LEU:HD21	1.93	0.50
1:A:1408:ARG:O	1:A:1412:HIS:HB2	2.11	0.50
1:A:1091:LEU:HD21	1:A:1614:GLU:HA	1.93	0.50
1:A:1618:SER:HA	1:A:1621:MET:HE3	1.94	0.50
1:B:1066:MET:HE2	1:B:1652:PHE:HB2	1.93	0.49
1:B:1077:LEU:HD13	1:B:1674:ILE:HD11	1.93	0.49
1:D:2221:TRP:CD1	1:D:2224:ARG:HH21	2.29	0.49
1:A:240:VAL:HB	1:A:431:ILE:HG23	1.94	0.49
1:B:819:ILE:HG22	1:B:820:THR:HG23	1.94	0.49
1:B:1939:PHE:O	1:B:1943:GLN:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1982:VAL:HG11	1:C:2036:LEU:HD23	1.95	0.49
1:D:2196:PHE:O	1:D:2200:THR:HG23	2.12	0.49
1:A:1219:LEU:O	1:A:1222:ILE:HG12	2.13	0.49
1:B:2200:THR:HA	1:B:2203:LEU:HD12	1.95	0.49
1:D:2304:LEU:HA	1:D:2307:THR:HG22	1.95	0.49
1:A:503:ARG:HD2	1:A:567:TYR:CE1	2.48	0.49
1:B:1797:LEU:HD22	1:B:1803:SER:HA	1.95	0.48
1:A:369:LEU:HD22	1:A:387:VAL:HG21	1.95	0.48
1:A:797:PRO:HB3	1:A:983:VAL:HG12	1.95	0.48
1:A:2422:THR:HG21	1:B:2471:TYR:CE2	2.49	0.48
1:B:1681:MET:HE2	1:B:1749:LEU:HD11	1.95	0.48
1:B:2207:MET:HE1	1:B:2597:VAL:HG21	1.96	0.48
1:A:842:LEU:O	1:A:846:VAL:HG13	2.13	0.48
1:B:1632:LEU:HD13	1:B:1652:PHE:CE2	2.48	0.48
1:B:1093:ALA:O	1:B:1097:VAL:HG13	2.12	0.48
1:B:1977:ILE:HD12	1:B:1985:VAL:HG21	1.95	0.48
1:A:509:MET:O	1:A:514:ILE:HG22	2.12	0.48
1:A:745:GLN:HG3	1:A:747:LEU:H	1.77	0.48
1:A:2196:PHE:O	1:A:2200:THR:HG23	2.13	0.48
1:A:1312:PHE:O	1:A:1316:ILE:HG23	2.14	0.48
1:B:2071:ARG:HD2	1:B:2125:MET:HE2	1.96	0.48
1:B:815:GLU:O	1:B:819:ILE:HG12	2.14	0.48
1:C:1973:LEU:O	1:C:1977:ILE:HG22	2.14	0.48
1:C:2181:PHE:HB2	1:C:2589:MET:HE1	1.96	0.48
1:C:2046:LYS:HB2	1:C:2046:LYS:HE3	1.76	0.47
1:A:800:TYR:HA	1:A:1097:VAL:HG12	1.96	0.47
1:A:2074:VAL:HA	1:A:2077:MET:HE2	1.96	0.47
1:B:872:ILE:HG12	1:B:882:LEU:HD21	1.96	0.47
1:C:1912:SER:HB3	1:C:1915:ILE:HG12	1.96	0.47
1:A:1421:ILE:HG13	1:A:1422:ALA:N	2.29	0.47
1:A:1996:CYS:SG	1:A:2007:ILE:HD12	2.54	0.47
1:A:882:LEU:O	1:A:886:THR:HG23	2.13	0.47
1:A:1761:VAL:HG13	1:A:1770:ILE:HG22	1.97	0.47
1:B:2181:PHE:HB2	1:B:2589:MET:HE1	1.96	0.47
1:B:2535:LEU:HD13	1:C:2384:VAL:HG12	1.96	0.47
1:C:2505:ARG:HG3	1:D:2426:ASP:HB2	1.96	0.47
1:A:1091:LEU:HD11	1:A:1613:LEU:HB3	1.97	0.47
1:A:1313:LEU:HD22	1:A:1331:VAL:HG22	1.96	0.47
1:A:1317:VAL:HG12	1:A:1327:CYS:HB3	1.95	0.47
1:A:2221:TRP:HD1	1:A:2224:ARG:HH12	1.63	0.47
1:B:2065:LEU:HG	1:B:2115:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:466:GLN:HG2	1:A:470:ARG:HE	1.80	0.47
1:B:1228:ASP:O	1:B:1229:GLU:HG2	2.14	0.47
1:B:1610:VAL:O	1:B:1614:GLU:HG3	2.15	0.47
1:B:1657:ILE:HA	1:B:1660:THR:HG22	1.96	0.47
1:B:978:GLN:HG2	1:B:1079:LEU:HD21	1.97	0.47
1:A:2631:ALA:HB3	1:A:2634:LEU:HG	1.96	0.46
1:C:2033:ARG:HB3	1:C:2036:LEU:HD13	1.97	0.46
1:A:518:VAL:O	1:A:521:ILE:HG22	2.15	0.46
1:A:1343:LEU:HD23	1:A:1378:LEU:HD21	1.97	0.46
1:A:1352:PHE:HE1	1:A:1409:VAL:HG22	1.80	0.46
1:B:992:MET:O	1:B:995:ILE:HG22	2.15	0.46
1:C:2207:MET:HE1	1:C:2597:VAL:HG21	1.97	0.46
1:A:1926:GLN:HG3	1:A:1994:GLU:HG3	1.97	0.46
1:B:1660:THR:HA	1:B:1663:LEU:HB2	1.97	0.46
1:A:2210:GLN:O	1:A:2214:ARG:HG2	2.16	0.46
1:B:1663:LEU:HD22	1:B:1667:GLU:HB2	1.97	0.46
1:B:2196:PHE:O	1:B:2200:THR:HG23	2.15	0.46
1:A:363:ILE:HG13	1:A:393:CYS:HB2	1.98	0.46
1:A:1351:SER:O	1:A:1354:ILE:HG12	2.16	0.46
1:A:1929:CYS:SG	1:A:1940:LEU:HD22	2.56	0.46
1:B:1066:MET:HE1	1:B:1649:CYS:SG	2.56	0.46
1:A:253:CYS:HB3	1:A:307:HIS:CD2	2.50	0.46
1:B:1982:VAL:HG11	1:B:2036:LEU:HD13	1.98	0.46
1:D:2229:TRP:HB3	1:D:2322:PHE:HB2	1.98	0.46
1:A:1246:CYS:SG	1:A:1256:LEU:HD12	2.56	0.46
1:A:2184:THR:HG23	1:A:2195:ASP:HB2	1.97	0.46
1:A:837:PHE:O	1:A:840:GLU:HG3	2.15	0.45
1:C:1996:CYS:HB3	1:C:2004:GLN:HG2	1.98	0.45
1:C:2209:TRP:CE3	1:C:2334:THR:HG22	2.51	0.45
1:D:2332:THR:HG22	1:D:2340:VAL:HG22	1.97	0.45
1:A:602:ASN:HB3	1:A:605:LEU:HB2	1.98	0.45
1:B:2508:SER:HB3	1:B:2511:GLU:HG3	1.99	0.45
1:C:2196:PHE:O	1:C:2200:THR:HG23	2.16	0.45
1:C:2575:LYS:HE2	1:C:2634:LEU:HD13	1.99	0.45
1:A:391:HIS:HE1	1:A:393:CYS:HB3	1.81	0.45
1:A:571:GLN:HG2	1:A:598:LEU:HD12	1.99	0.45
1:B:1246:CYS:SG	1:B:1256:LEU:HD12	2.55	0.45
1:A:1769:ARG:O	1:A:1773:GLU:HG2	2.17	0.45
1:A:1099:LEU:HD22	1:A:1606:LEU:HD22	1.99	0.45
1:B:2184:THR:HG23	1:B:2195:ASP:HB3	1.99	0.45
1:A:410:GLU:HG3	1:A:411:ARG:H	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1264:LEU:HD23	1:A:1264:LEU:HA	1.87	0.45
1:C:1782:LEU:HD11	1:C:1790:GLN:HG3	1.98	0.45
1:B:1224:TYR:HB2	1:B:1231:MET:HG3	1.99	0.45
1:D:2319:LYS:HD2	1:D:2319:LYS:HA	1.79	0.45
1:A:1230:LYS:O	1:A:1233:GLU:HG2	2.18	0.44
1:D:2235:ASN:HD21	1:D:2288:ARG:HD3	1.83	0.44
1:A:547:ALA:N	1:A:548:PRO:HD2	2.32	0.44
1:A:716:ALA:HB1	1:A:724:LEU:HD13	1.99	0.44
1:B:1684:LYS:HD2	1:B:1684:LYS:HA	1.77	0.44
1:B:2598:LEU:O	1:B:2602:LYS:HB2	2.16	0.44
1:B:1624:GLU:HB3	1:B:1695:LEU:HD21	1.99	0.44
1:C:1792:SER:HA	1:C:1795:GLN:HG2	2.00	0.44
1:B:2069:ARG:HB3	1:B:2072:GLU:HG3	1.98	0.44
1:B:2589:MET:HE3	1:B:2590:TRP:CE2	2.53	0.44
1:B:1929:CYS:SG	1:B:1940:LEU:HD22	2.58	0.44
1:D:2420:ASP:OD2	1:D:2517:ARG:HD3	2.18	0.44
1:C:2069:ARG:HB2	1:C:2072:GLU:HB2	2.00	0.44
1:C:2153:ARG:HB2	1:C:2157:THR:HG22	2.00	0.44
1:A:2359:GLY:HA2	1:A:2363:HIS:O	2.18	0.44
1:B:1278:PHE:HE1	1:B:1284:LEU:HD22	1.82	0.44
1:C:2106:HIS:CE1	1:C:2164:PRO:HB3	2.53	0.44
1:A:302:LEU:HB3	1:A:366:LEU:HD22	1.99	0.43
1:B:2042:ASN:HB2	1:B:2104:VAL:HG22	1.99	0.43
1:D:2319:LYS:HG3	1:D:2353:VAL:HG22	2.00	0.43
1:A:1974:GLY:HA2	1:A:2026:ILE:HG23	2.00	0.43
1:B:1055:ARG:HH11	1:B:1059:ARG:HH21	1.66	0.43
1:B:1767:ASN:HD21	1:B:1769:ARG:NH2	2.16	0.43
1:B:2413:GLY:HA2	1:B:2417:LEU:HB2	2.00	0.43
1:D:2359:GLY:HA2	1:D:2363:HIS:O	2.18	0.43
1:C:2602:LYS:HB3	1:C:2607:TYR:HE1	1.83	0.43
1:A:838:VAL:HG11	1:A:868:ALA:HB2	2.01	0.43
1:A:1073:LEU:HG	1:A:1659:HIS:CE1	2.53	0.43
1:B:804:TRP:CE3	1:B:1099:LEU:HD12	2.54	0.43
1:A:226:TYR:C	1:A:228:SER:H	2.25	0.43
1:A:304:ARG:HG2	1:A:365:SER:O	2.19	0.43
1:A:2426:ASP:HB2	1:D:2505:ARG:HG3	2.00	0.43
1:A:2029:LEU:HD11	1:A:2036:LEU:HD12	2.00	0.43
1:B:2567:LEU:HD23	1:B:2567:LEU:HA	1.81	0.43
1:C:1977:ILE:HG21	1:C:2026:ILE:HD13	2.01	0.43
1:C:2613:TYR:HE1	1:C:2617:MET:HE3	1.83	0.43
1:A:2471:TYR:CE2	1:D:2422:THR:HG21	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1689:VAL:HG22	1:B:1690:GLU:H	1.83	0.43
1:A:509:MET:SD	1:A:514:ILE:HG21	2.59	0.43
1:A:1324:VAL:HG12	1:A:1327:CYS:H	1.83	0.43
1:A:1946:LYS:HE2	1:A:1946:LYS:HB2	1.89	0.43
1:B:2547:LEU:O	1:B:2550:GLU:HG3	2.18	0.43
1:A:578:PHE:CZ	1:A:599:LEU:HD11	2.54	0.43
1:B:1129:TRP:HA	1:B:1175:LYS:HD3	2.00	0.43
1:C:2027:ASN:HB2	1:C:2028:PRO:HD3	2.01	0.43
1:C:2119:ASN:HB3	1:C:2122:LEU:HB3	2.01	0.43
1:A:229:TYR:HA	1:A:235:LYS:HD3	2.00	0.43
1:A:435:PRO:O	1:A:439:VAL:HG23	2.19	0.43
1:A:727:LEU:HD23	1:A:727:LEU:HA	1.90	0.43
1:A:2509:LYS:HD2	1:B:2484:MET:HE2	2.00	0.43
1:C:1959:LEU:HB2	1:C:1988:ASN:CG	2.43	0.43
1:D:2297:ARG:HD2	1:D:2297:ARG:HA	1.85	0.43
1:A:612:ALA:HA	1:A:651:LEU:HD21	2.01	0.42
1:A:2319:LYS:HA	1:A:2319:LYS:HD2	1.73	0.42
1:B:1239:HIS:CD2	1:B:1269:LEU:HB3	2.54	0.42
1:B:1255:LEU:HD23	1:B:1255:LEU:HA	1.88	0.42
1:B:1761:VAL:HG13	1:B:1770:ILE:HG22	2.00	0.42
1:C:1919:GLN:HB3	1:C:1920:PRO:HD3	2.01	0.42
1:C:2229:TRP:HB2	1:C:2322:PHE:HD2	1.84	0.42
1:C:2413:GLY:HA2	1:C:2417:LEU:HB2	2.00	0.42
1:D:2588:ASN:HB3	1:D:2591:HIS:CG	2.54	0.42
1:A:803:LEU:HD11	1:A:1106:VAL:HG22	2.01	0.42
1:D:2221:TRP:HD1	1:D:2224:ARG:HH21	1.67	0.42
1:A:1196:ASN:HD21	1:A:1198:LYS:HB3	1.84	0.42
1:B:879:PHE:HE1	1:B:983:VAL:HG23	1.83	0.42
1:B:1126:SER:HA	1:B:1129:TRP:CD1	2.54	0.42
1:B:2537:PHE:HB3	1:C:2537:PHE:HZ	1.83	0.42
1:A:2184:THR:HG22	1:A:2192:LYS:HB3	2.01	0.42
1:B:745:GLN:HG2	1:B:747:LEU:H	1.85	0.42
1:D:2343:ASP:O	1:D:2347:LEU:HG	2.20	0.42
1:A:1297:VAL:HG21	1:A:1334:GLU:HB3	2.02	0.42
1:B:772:PHE:HB2	1:B:856:GLU:HG3	2.00	0.42
1:B:966:VAL:HG12	1:B:970:LYS:HD2	2.01	0.42
1:B:1673:LYS:HD3	1:B:1673:LYS:HA	1.85	0.42
1:B:1796:GLN:O	1:B:1800:GLN:HB2	2.19	0.42
1:B:2210:GLN:HA	1:B:2213:ILE:HG22	2.01	0.42
1:B:2299:ILE:HG13	1:B:2307:THR:HG21	2.02	0.42
1:A:394:THR:O	1:A:396:THR:HG23	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:MET:O	1:A:995:ILE:HG22	2.20	0.42
1:A:1689:VAL:HG22	1:A:1690:GLU:H	1.84	0.42
1:B:2239:PHE:HB3	1:B:2295:MET:SD	2.60	0.42
1:B:2298:SER:O	1:B:2302:ILE:HG22	2.20	0.42
1:A:627:GLU:HB2	1:A:630:PHE:HD2	1.83	0.42
1:A:1065:ILE:HA	1:A:1073:LEU:HD13	2.02	0.42
1:B:2026:ILE:HD12	1:B:2037:VAL:HG13	2.02	0.42
1:C:2579:PHE:CE2	1:C:2583:ILE:HD12	2.54	0.42
1:A:811:ILE:HD11	1:A:816:TYR:HB2	2.01	0.42
1:A:1392:TYR:O	1:A:1396:LYS:HG3	2.20	0.42
1:B:968:ASP:O	1:B:972:LYS:HG2	2.20	0.42
1:B:1786:ASN:HB3	1:B:1789:THR:OG1	2.19	0.42
1:B:2204:TYR:HA	1:B:2207:MET:HE3	2.02	0.42
1:C:2148:GLN:HB2	1:C:2160:GLN:HE21	1.84	0.42
1:D:2507:PRO:HD3	1:D:2517:ARG:HH21	1.84	0.42
1:A:350:ILE:HD12	1:A:418:GLY:HA3	2.02	0.42
1:B:1065:ILE:HG21	1:B:1652:PHE:HE1	1.84	0.42
1:B:2077:MET:HE1	1:B:2139:LEU:HD22	2.02	0.42
1:A:1181:ILE:O	1:A:1185:ILE:HG12	2.20	0.41
1:A:1786:ASN:HB3	1:A:1789:THR:OG1	2.20	0.41
1:B:2319:LYS:HG3	1:B:2353:VAL:HG22	2.02	0.41
1:C:2172:LEU:HD11	1:C:2203:LEU:HD22	2.02	0.41
1:A:599:LEU:O	1:A:606:LEU:HD12	2.19	0.41
1:A:843:LYS:O	1:A:846:VAL:HG22	2.21	0.41
1:A:2308:LEU:HD12	1:A:2308:LEU:HA	1.94	0.41
1:A:2595:PHE:HE2	1:A:2614:VAL:HG21	1.84	0.41
1:B:1216:VAL:HG21	1:B:1241:PHE:CD2	2.55	0.41
1:B:1218:ASP:O	1:B:1222:ILE:HG23	2.21	0.41
1:B:1623:ALA:HB3	1:B:1695:LEU:HD23	2.02	0.41
1:B:1635:PRO:HG3	1:B:1652:PHE:CD2	2.55	0.41
1:C:1797:LEU:HD23	1:C:1797:LEU:HA	1.94	0.41
1:A:872:ILE:HG12	1:A:882:LEU:HD21	2.02	0.41
1:A:886:THR:HG22	1:A:980:ILE:HD13	2.02	0.41
1:B:1620:MET:HE3	1:B:1691:GLU:HB2	2.02	0.41
1:A:1077:LEU:HD21	1:A:1656:LEU:HD11	2.01	0.41
1:A:2384:VAL:HG12	1:D:2535:LEU:HD13	2.01	0.41
1:B:2349:HIS:O	1:B:2353:VAL:HG23	2.20	0.41
1:B:2564:ILE:HD11	1:B:2589:MET:HB3	2.01	0.41
1:C:2219:LEU:HD12	1:C:2219:LEU:HA	1.94	0.41
1:B:2523:LEU:HD23	1:B:2523:LEU:HA	1.89	0.41
1:A:1356:LEU:HD22	1:A:1414:ASP:HB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2523:LEU:HD23	1:D:2523:LEU:HA	1.89	0.41
1:A:406:ASP:HB2	1:A:409:GLU:HB2	2.03	0.41
1:A:457:LYS:HE2	1:A:457:LYS:HB2	1.90	0.41
1:A:482:PHE:HE2	1:A:509:MET:HE3	1.86	0.41
1:B:668:THR:HG22	1:B:760:LEU:HD11	2.01	0.41
1:C:2071:ARG:NH1	1:C:2125:MET:HE2	2.36	0.41
1:C:2505:ARG:HD3	1:D:2471:TYR:CZ	2.56	0.41
1:A:573:TYR:HA	1:A:576:LYS:HE2	2.02	0.41
1:A:644:ALA:HB2	1:A:742:LEU:HD23	2.02	0.41
1:A:1193:CYS:O	1:A:1200:ARG:HG3	2.21	0.41
1:A:1255:LEU:HD23	1:A:1255:LEU:HA	1.88	0.41
1:A:1397:CYS:HA	1:A:1400:LEU:HB2	2.03	0.41
1:A:2194:ASN:O	1:A:2198:GLN:HG2	2.20	0.41
1:A:235:LYS:HE2	1:A:235:LYS:HB2	1.95	0.41
1:A:595:ILE:HD13	1:A:595:ILE:HA	1.95	0.41
1:A:596:THR:HG21	1:A:633:TYR:CD1	2.56	0.41
1:A:1617:PHE:HB3	1:A:1621:MET:HE2	2.03	0.41
1:A:2073:LEU:O	1:A:2076:VAL:HG12	2.20	0.41
1:B:807:ILE:HD13	1:B:993:LEU:HB3	2.03	0.41
1:B:2589:MET:HE3	1:B:2590:TRP:NE1	2.36	0.41
1:C:1800:GLN:HB3	1:C:1802:LYS:HG3	2.03	0.41
1:C:1805:LYS:HA	1:C:1805:LYS:HD2	1.83	0.41
1:C:1820:GLU:HB2	1:C:1915:ILE:HD11	2.03	0.41
1:A:302:LEU:HD23	1:A:366:LEU:HB3	2.02	0.41
1:A:1633:TYR:HE2	1:A:1740:ILE:HD13	1.85	0.41
1:B:1195:GLN:HG3	1:B:1196:ASN:H	1.86	0.41
1:B:1245:PHE:CE2	1:B:1252:ASN:HB3	2.56	0.41
1:B:1647:ILE:HD12	1:B:1647:ILE:HA	1.90	0.41
1:B:1758:VAL:O	1:B:1762:ILE:HG12	2.20	0.41
1:B:1762:ILE:HG23	1:B:1771:PHE:HE1	1.85	0.41
1:B:1928:LEU:HD23	1:B:1928:LEU:HA	1.92	0.41
1:C:1921:ILE:O	1:C:1925:LEU:HG	2.21	0.41
1:D:2603:ASP:HB3	1:D:2606:GLU:OE1	2.20	0.41
1:A:1919:GLN:HB3	1:A:1920:PRO:HD3	2.04	0.40
1:C:2506:ARG:HE	1:C:2506:ARG:HB2	1.70	0.40
1:A:1409:VAL:HG11	1:A:1423:TYR:CE2	2.56	0.40
1:A:2422:THR:HG21	1:B:2471:TYR:HE2	1.86	0.40
1:B:653:CYS:SG	1:B:748:ALA:HB2	2.61	0.40
1:B:666:ILE:HG12	1:B:697:TRP:HB3	2.03	0.40
1:D:2158:MET:HE2	1:D:2158:MET:HB3	2.00	0.40
1:A:1119:LEU:HB2	1:A:1185:ILE:HG21	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2210:GLN:O	1:D:2214:ARG:HG2	2.21	0.40
1:D:2589:MET:HE3	1:D:2590:TRP:CE2	2.56	0.40
1:A:239:VAL:HG21	1:A:439:VAL:HG22	2.03	0.40
1:A:1683:GLU:HB3	1:A:1685:LYS:HE2	2.03	0.40
1:A:2576:THR:HG23	1:A:2577:VAL:HG23	2.04	0.40
1:A:2617:MET:HE1	1:A:2624:ASP:HB2	2.03	0.40
1:B:890:LEU:HD22	1:B:1060:VAL:HG21	2.03	0.40
1:B:1220:LEU:HD23	1:B:1235:MET:SD	2.61	0.40
1:B:2422:THR:HG21	1:C:2471:TYR:CE2	2.56	0.40
1:A:401:THR:HB	1:A:403:ILE:HD12	2.02	0.40
1:B:1264:LEU:HD23	1:B:1264:LEU:HA	1.84	0.40
1:C:2557:ILE:O	1:C:2561:THR:HB	2.21	0.40
1:C:2583:ILE:HD11	3:C:2801:ATP:C2	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	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
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. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	421	GLN
1	A	517	GLN
1	A	786	HIS
1	A	1204	GLN
1	A	1232	ASN
1	A	1453	ASN
1	A	1800	GLN
1	A	1932	HIS
1	A	1957	GLN
1	A	1997	GLN
1	A	2056	HIS
1	A	2060	ASN
1	A	2118	HIS
1	A	2154	HIS
1	A	2199	GLN
1	A	2216	ASN
1	A	2318	ASN
1	B	1118	GLN

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Mol	Chain	Res	Type
1	B	1195	GLN
1	B	1306	HIS
1	B	1933	ASN
1	B	2004	GLN
1	B	2189	GLN
1	B	2216	ASN
1	C	1764	ASN
1	C	1767	ASN
1	C	1943	GLN
1	C	1948	ASN
1	C	1997	GLN
1	C	2067	ASN
1	C	2160	GLN
1	C	2194	ASN
1	C	2318	ASN
1	C	2574	ASN
1	D	2154	HIS
1	D	2189	GLN
1	D	2235	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.

All (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
3	C	2801	ATP	PB-O3A-PA-O1A

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Mol	Chain	Res	Type	Atoms
3	A	2802	ATP	PB-O3A-PA-O5'
3	D	2801	ATP	PB-O3A-PA-O5'
3	B	2801	ATP	PG-O3B-PB-O1B
3	A	2802	ATP	C5'-O5'-PA-O1A
3	C	2801	ATP	C5'-O5'-PA-O1A
3	D	2801	ATP	C5'-O5'-PA-O1A
2	A	2801	I3P	C4-O4-P4-O43
3	D	2801	ATP	O4'-C4'-C5'-O5'
3	A	2802	ATP	PB-O3B-PG-O1G
3	C	2801	ATP	PG-O3B-PB-O3A
3	D	2801	ATP	PB-O3B-PG-O3G
3	C	2801	ATP	PG-O3B-PB-O1B
3	C	2801	ATP	PB-O3A-PA-O2A
2	A	2801	I3P	C1-O1-P1-O13
3	C	2801	ATP	PG-O3B-PB-O2B

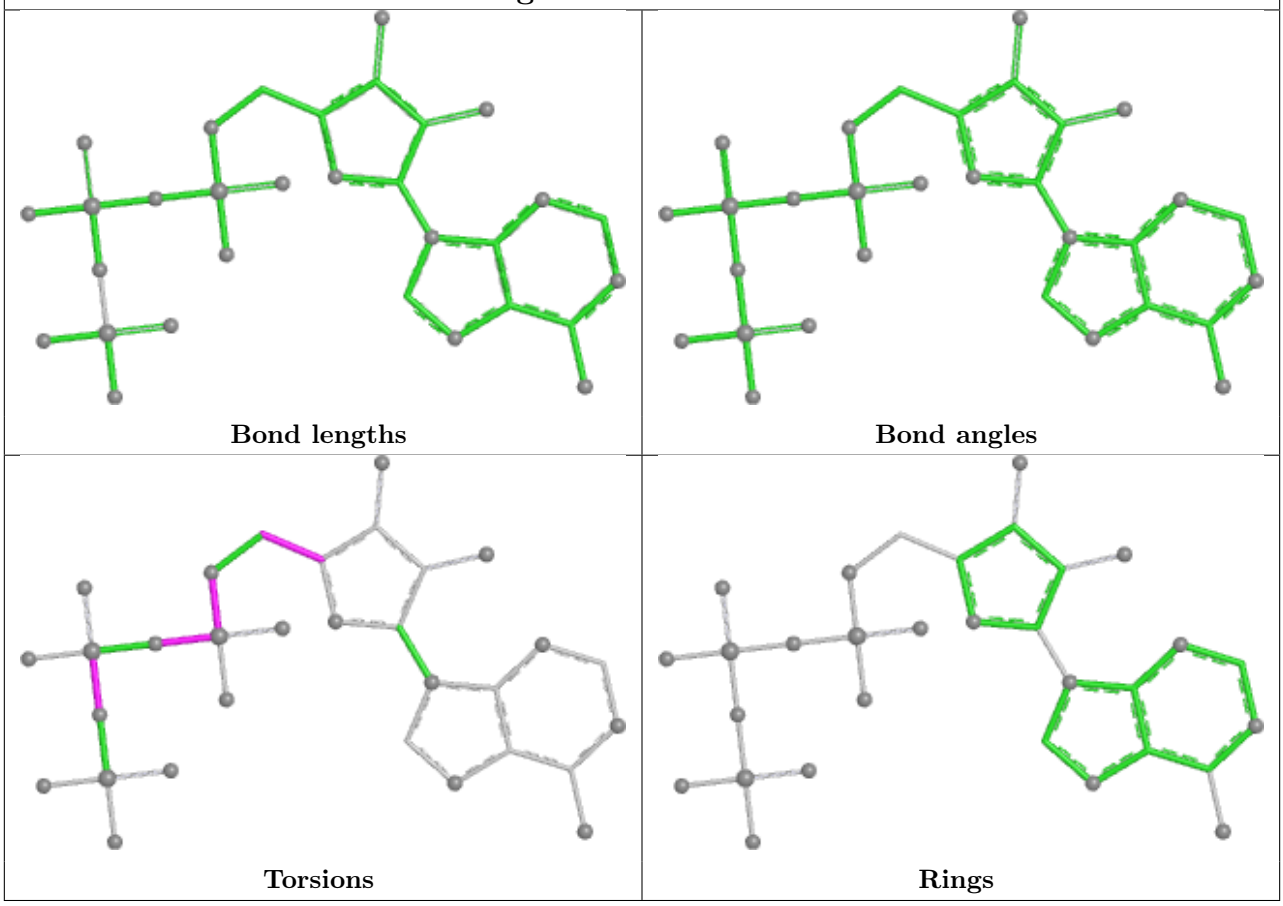
There are no ring outliers.

1 monomer is involved in 1 short contact:

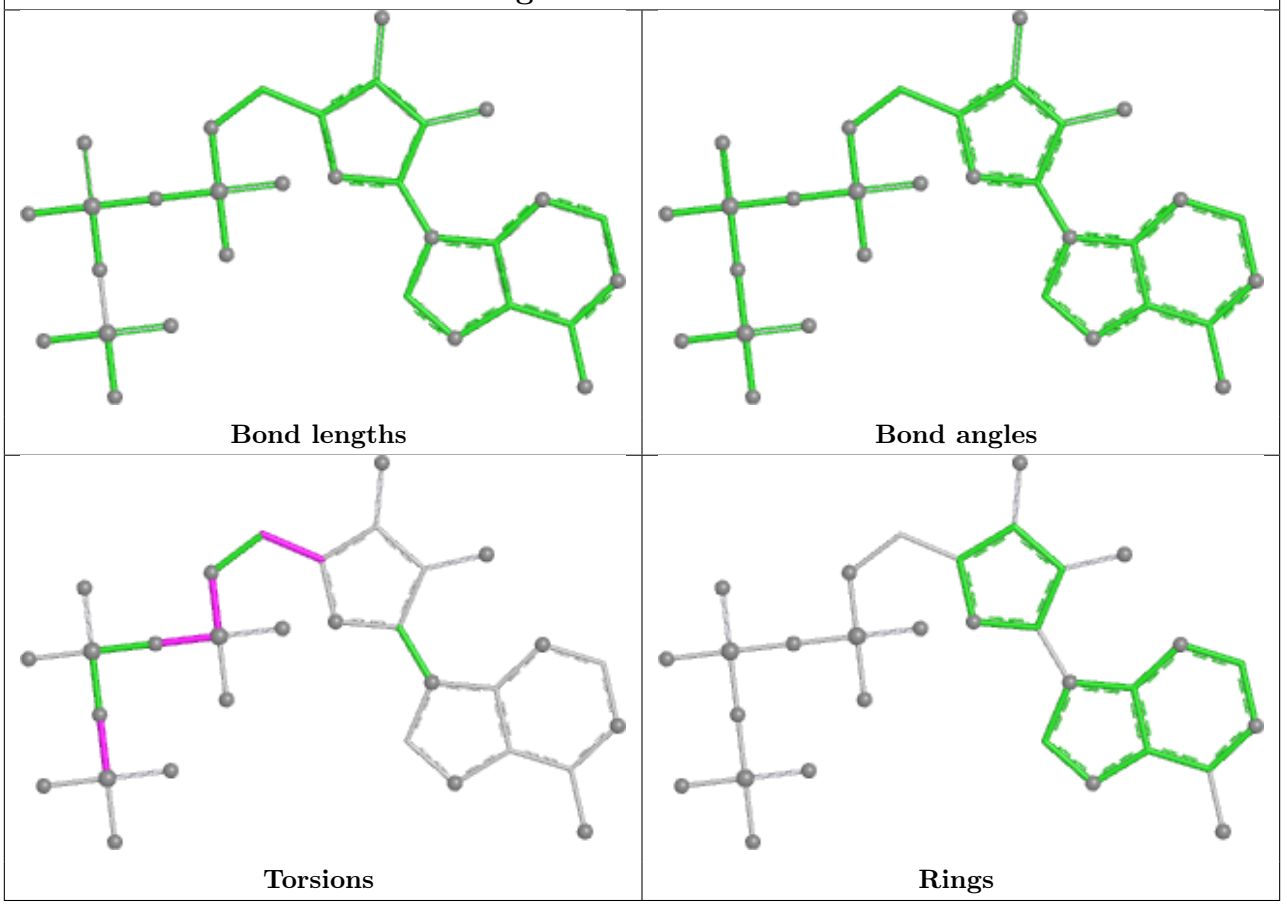
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	2801	ATP	1	0

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.

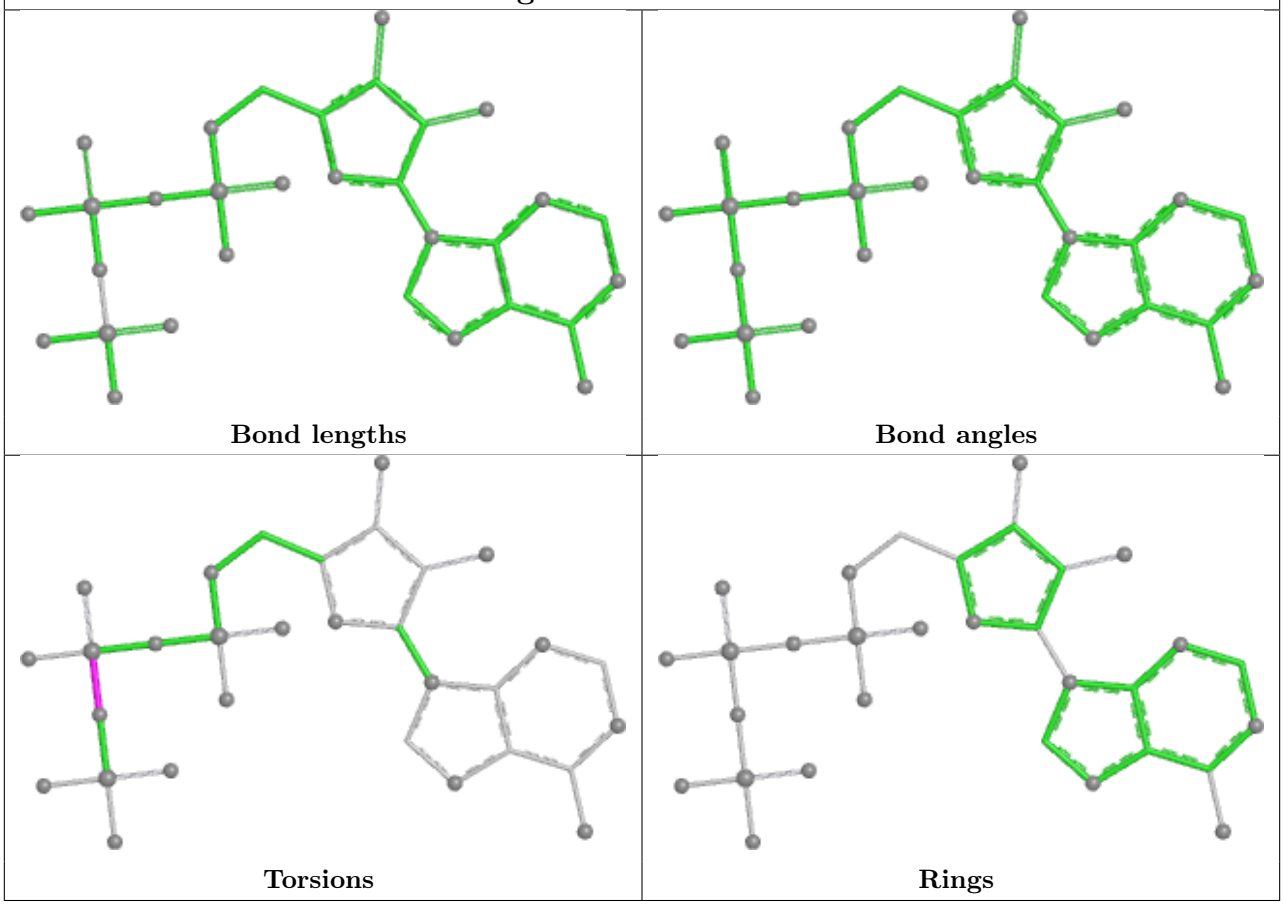
Ligand ATP C 2801



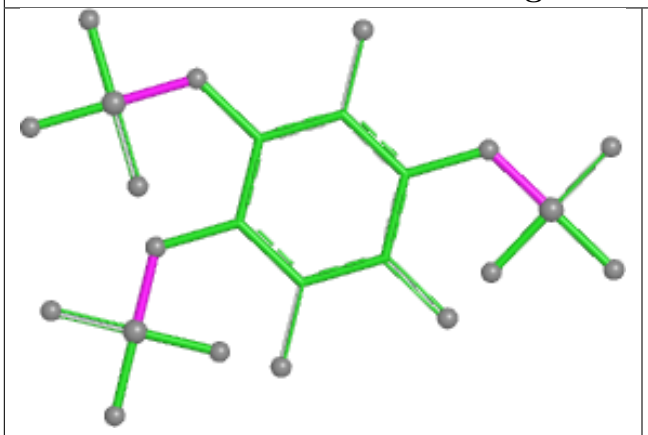
Ligand ATP D 2801



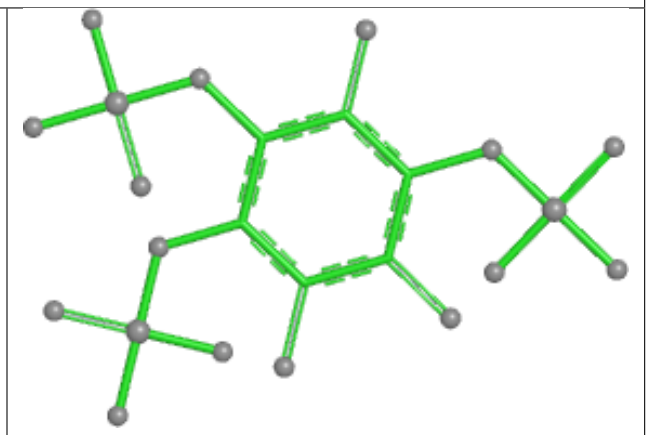
Ligand ATP B 2801



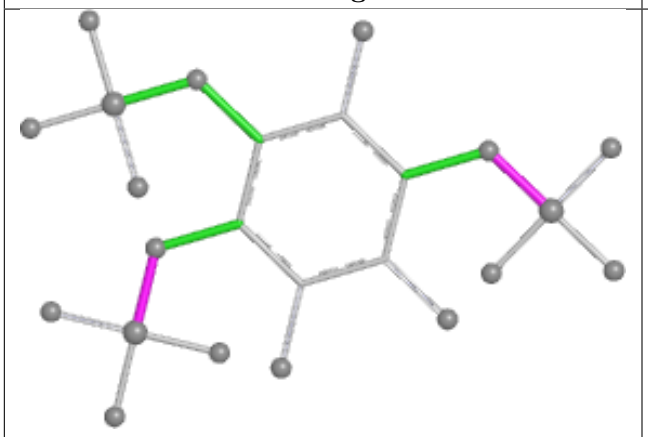
Ligand I3P A 2801



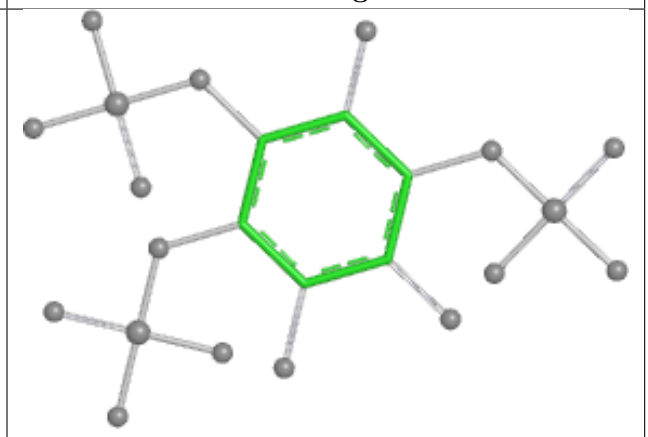
Bond lengths



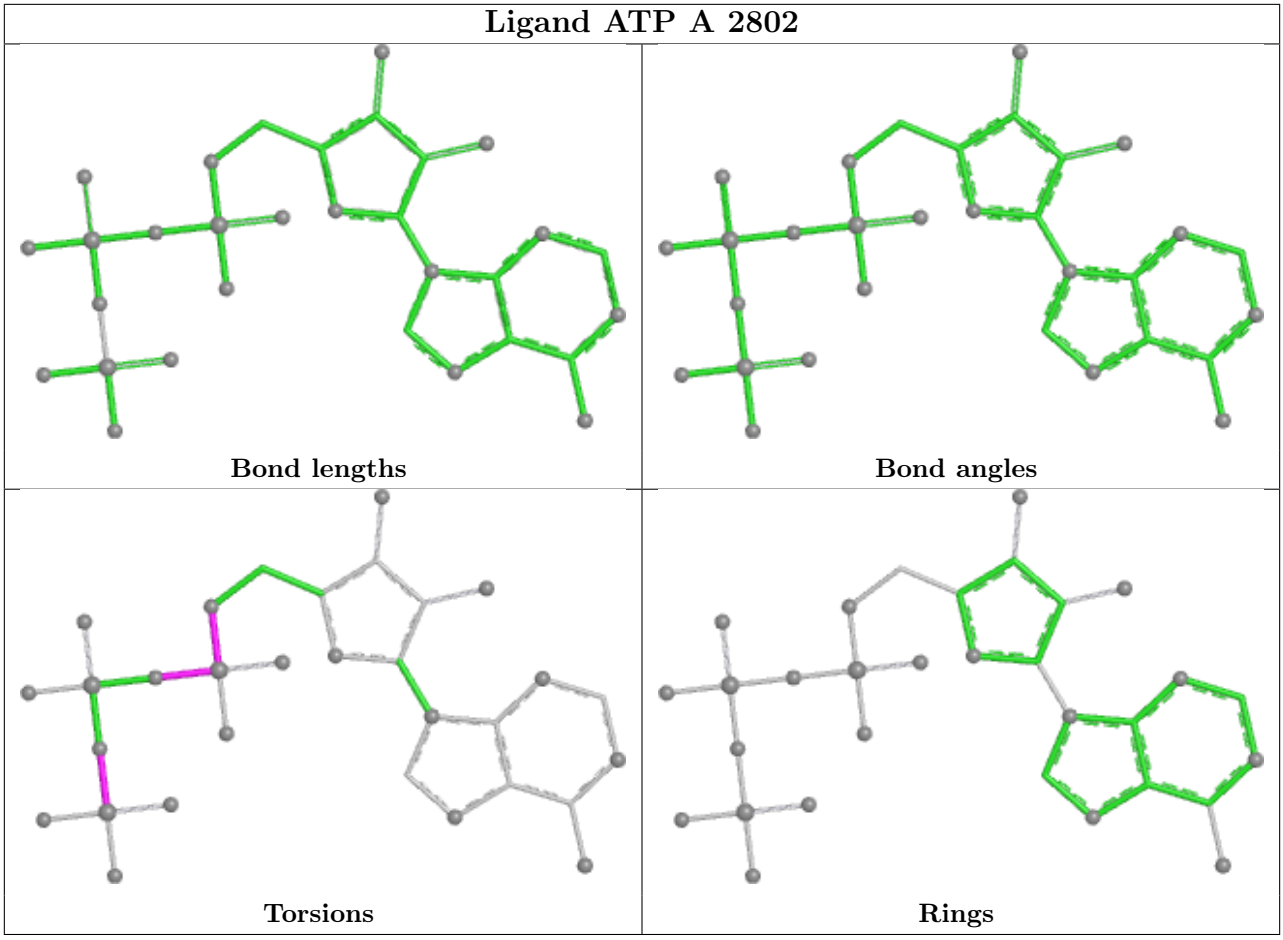
Bond angles



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.

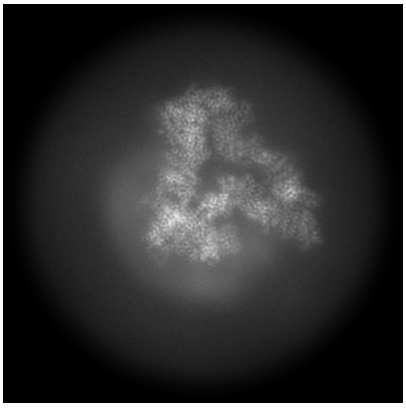
6 Map visualisation (i)

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.

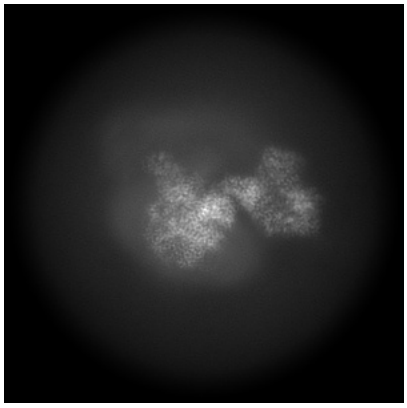
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

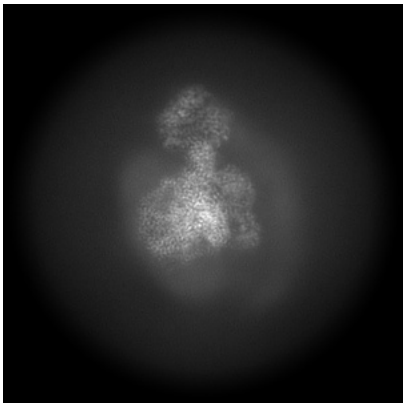
6.1.1 Primary map



X



Y

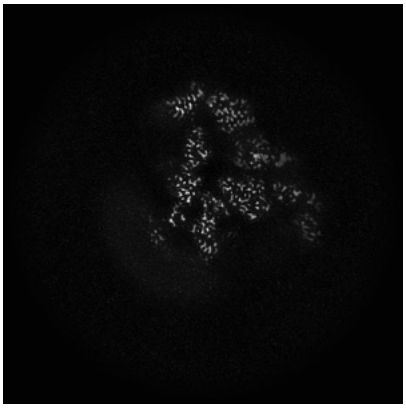


Z

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

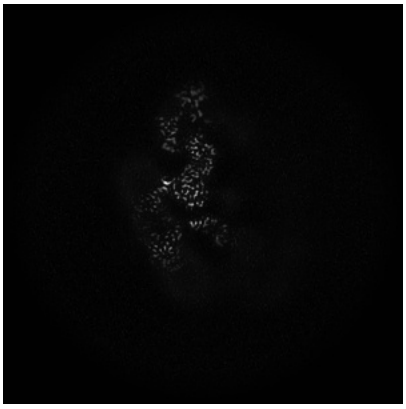
6.2 Central slices (i)

6.2.1 Primary map



X Index: 256

Y Index: 256

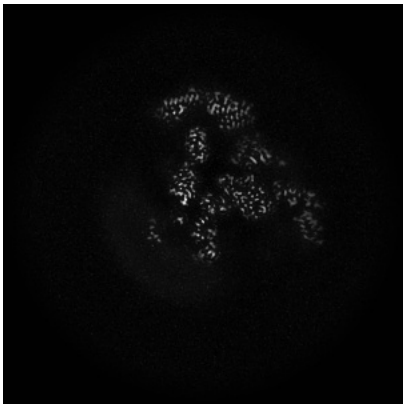


Z Index: 256

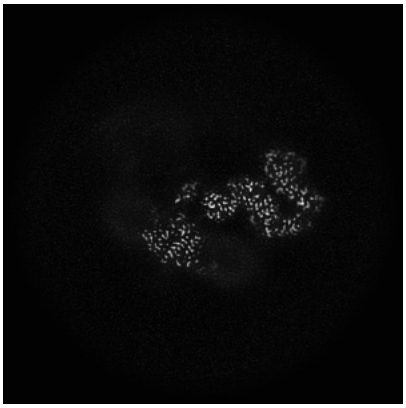
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

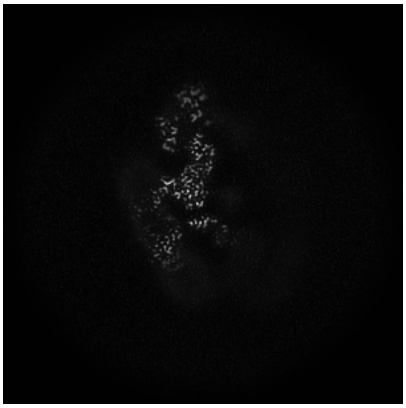
6.3.1 Primary map



X Index: 252



Y Index: 239

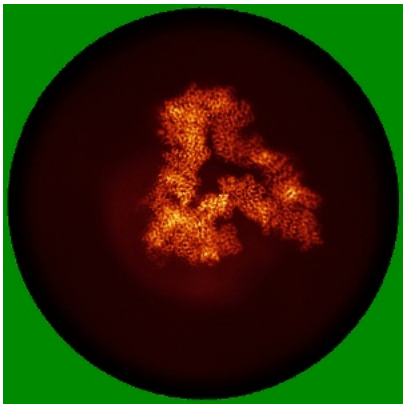


Z Index: 257

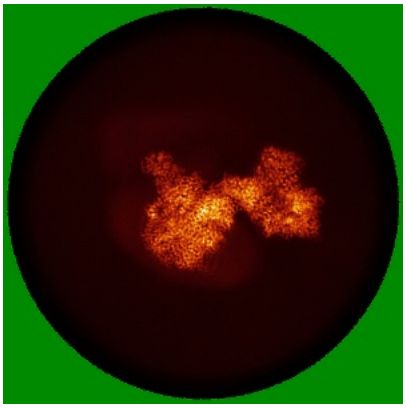
The images above show the largest variance slices of the map in three orthogonal directions.

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

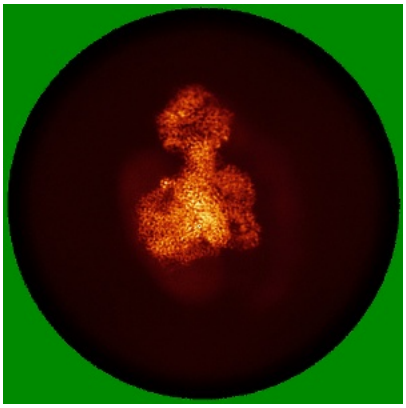
6.4.1 Primary map



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.

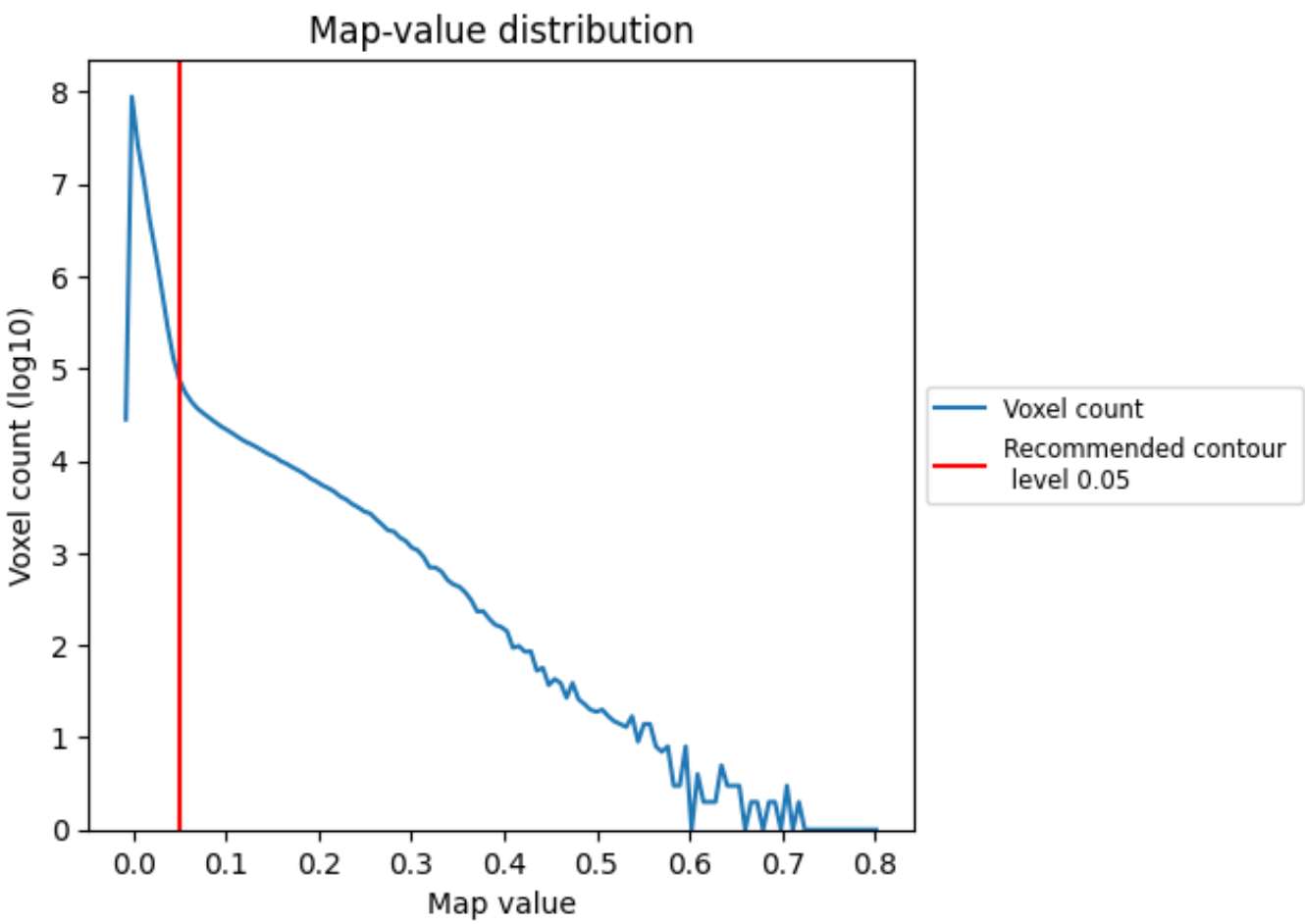
6.6 Mask visualisation (i)

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

7 Map analysis (i)

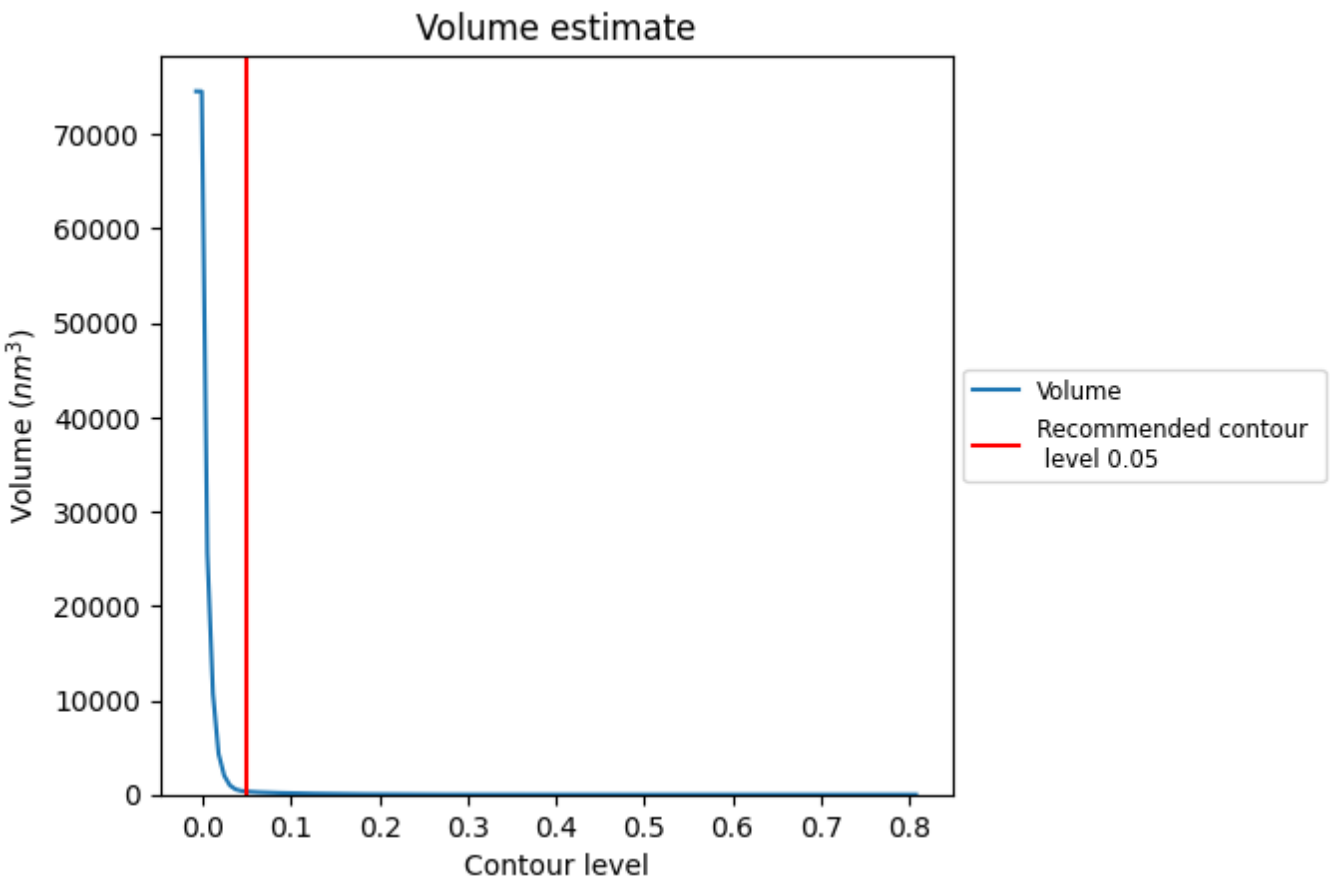
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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.

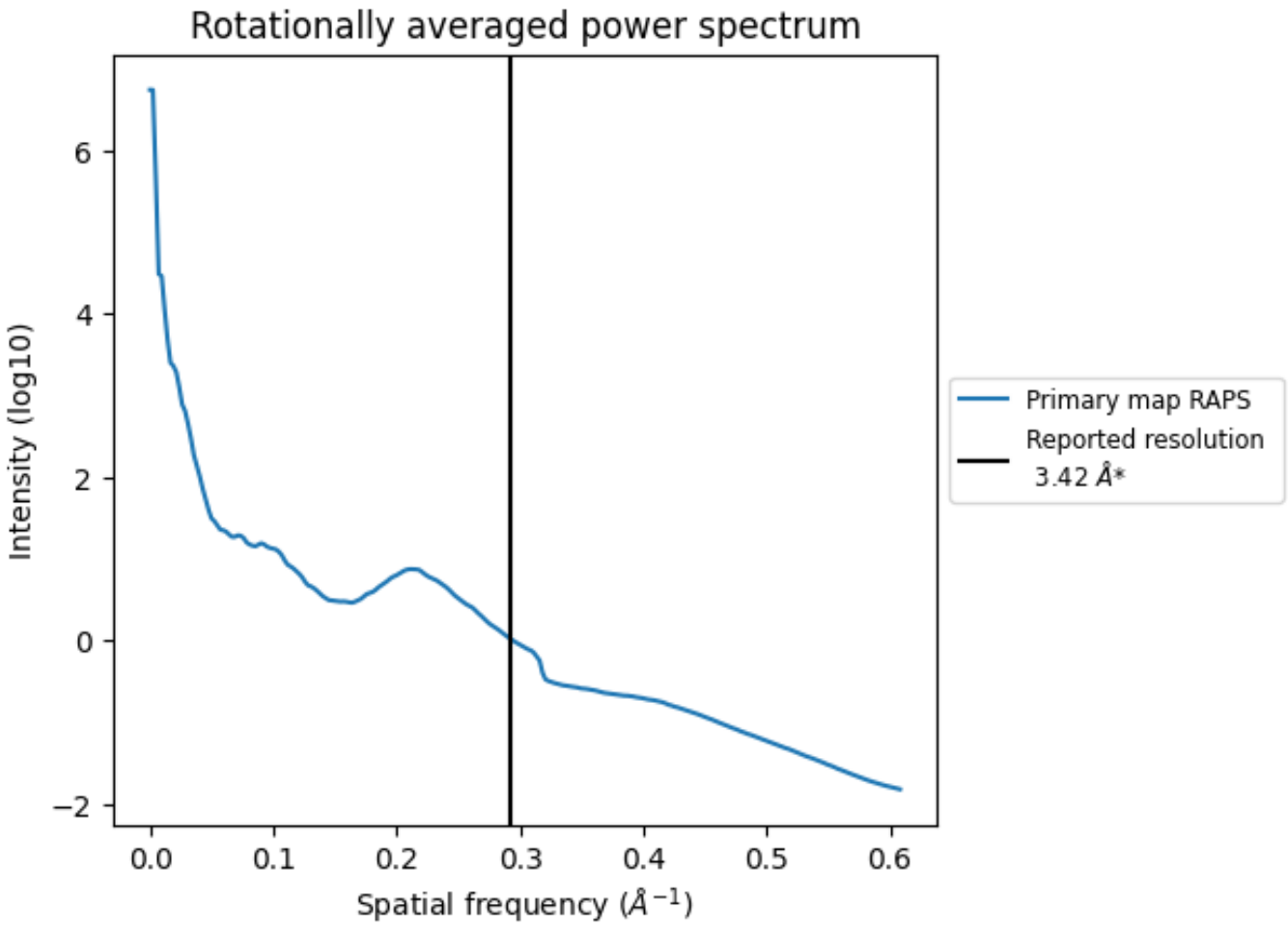
7.2 Volume estimate (i)



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}

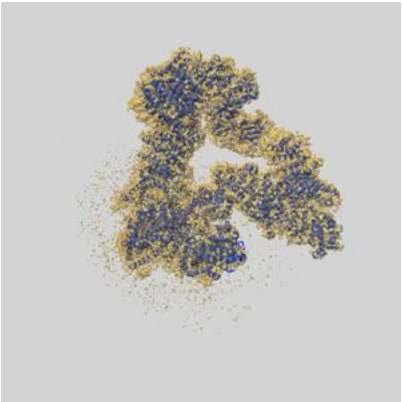
8 Fourier-Shell correlation (i)

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

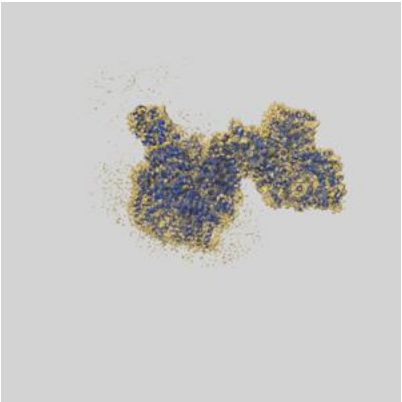
9 Map-model fit (i)

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.

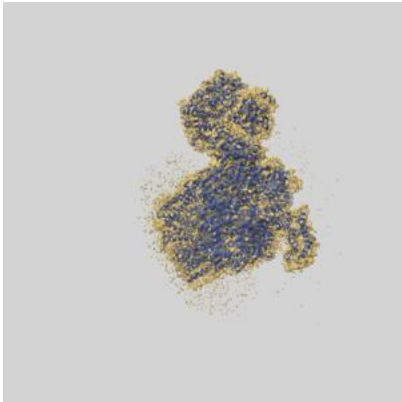
9.1 Map-model overlay (i)



X



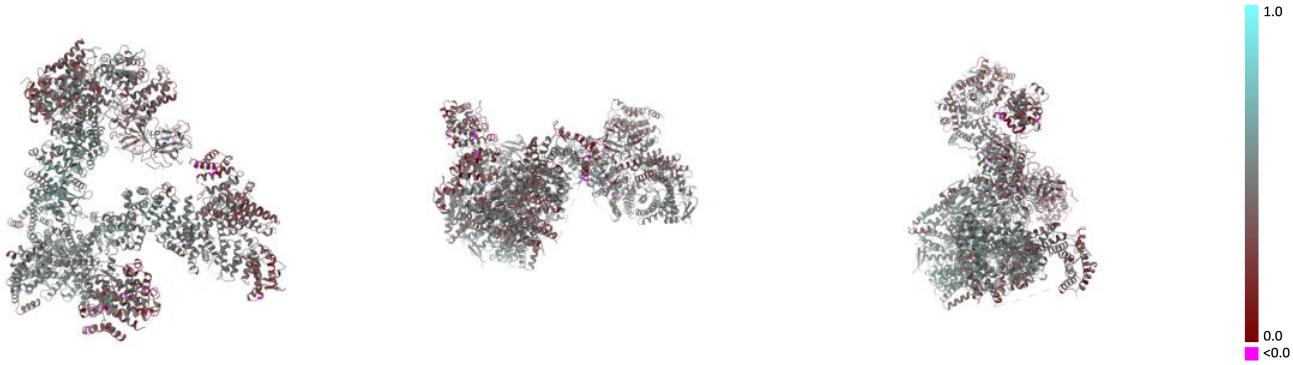
Y



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.

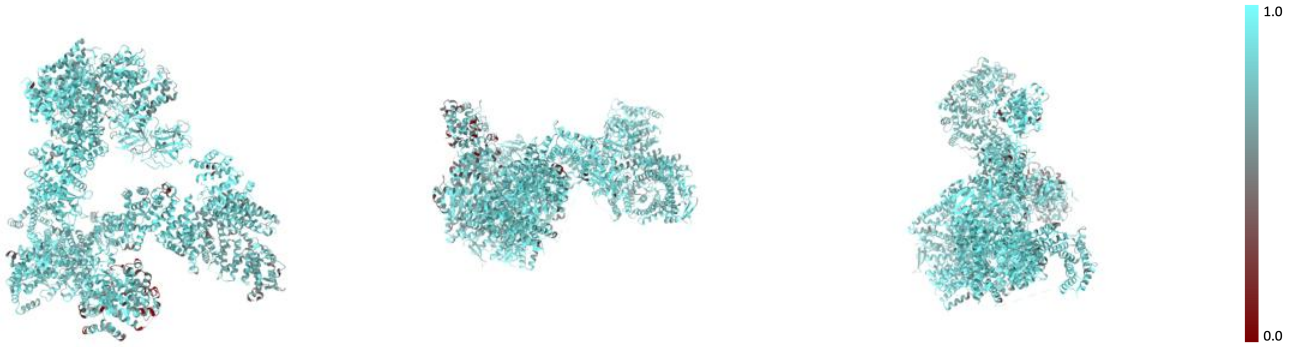
9.2 Q-score mapped to coordinate model (i)



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.

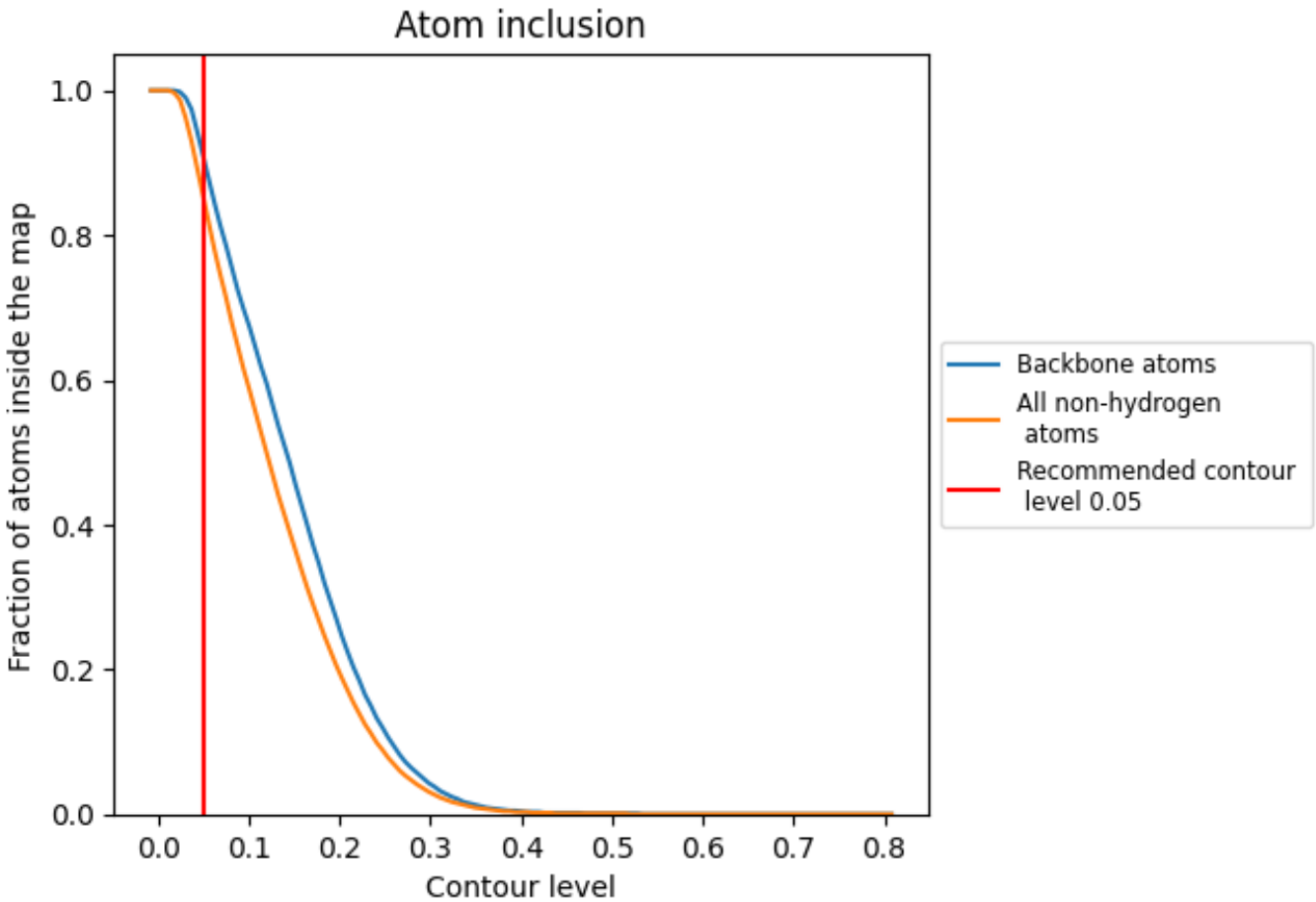
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.05).

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 (i)

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