



## Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 04:58 AM JST

PDB ID : 7EY5  
EMDB ID : EMD-31378  
Title : Local CryoEM structure of the SARS-CoV-2 S6PV2 in complex with BD-771 Fab and BD-821 Fab  
Authors : Zhang, Z.Y.  
Deposited on : 2021-05-29  
Resolution : 3.40 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](mailto: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.dev113  
MolProbity : 4.02b-467  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

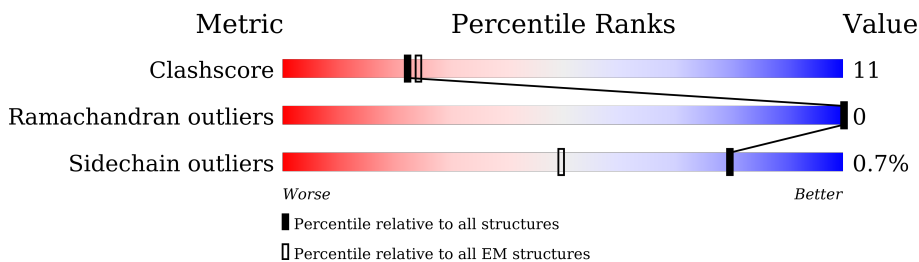
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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  $\geq 3$ , 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  $\leq 5\%$ . 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	1285	 12% 12% 12% 86%
2	B	231	 7% 33% 19% 48%
3	C	215	 7% 39% 11% 50%
4	H	241	 7% 40% 13% 46%
5	L	214	 7% 35% 15% 50%

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5072 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	183	Total	C	N	O	S	0	0
			1465	941	243	274	7		

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	21	PHE	LEU	conflict	UNP P0DTC2
A	83	ALA	ASP	conflict	UNP P0DTC2
A	218	GLY	ASP	conflict	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	ALA	deletion	UNP P0DTC2
A	417	ASN	LYS	conflict	UNP P0DTC2
A	484	LYS	GLU	conflict	UNP P0DTC2
A	501	TYR	ASN	conflict	UNP P0DTC2
A	614	GLY	ASP	conflict	UNP P0DTC2
A	682	GLY	ARG	conflict	UNP P0DTC2
A	683	SER	ARG	conflict	UNP P0DTC2
A	685	SER	ARG	conflict	UNP P0DTC2
A	701	VAL	ALA	conflict	UNP P0DTC2
A	817	PRO	PHE	conflict	UNP P0DTC2
A	892	PRO	ALA	conflict	UNP P0DTC2
A	899	PRO	ALA	conflict	UNP P0DTC2
A	942	PRO	ALA	conflict	UNP P0DTC2
A	986	PRO	LYS	conflict	UNP P0DTC2
A	987	PRO	VAL	conflict	UNP P0DTC2
A	1209	GLY	-	expression tag	UNP P0DTC2
A	1210	SER	-	expression tag	UNP P0DTC2
A	1211	GLY	-	expression tag	UNP P0DTC2
A	1212	TYR	-	expression tag	UNP P0DTC2
A	1213	ILE	-	expression tag	UNP P0DTC2
A	1214	PRO	-	expression tag	UNP P0DTC2
A	1215	GLU	-	expression tag	UNP P0DTC2
A	1216	ALA	-	expression tag	UNP P0DTC2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	1217	PRO	-	expression tag	UNP P0DTC2
A	1218	ARG	-	expression tag	UNP P0DTC2
A	1219	ASP	-	expression tag	UNP P0DTC2
A	1220	GLY	-	expression tag	UNP P0DTC2
A	1221	GLN	-	expression tag	UNP P0DTC2
A	1222	ALA	-	expression tag	UNP P0DTC2
A	1223	TYR	-	expression tag	UNP P0DTC2
A	1224	VAL	-	expression tag	UNP P0DTC2
A	1225	ARG	-	expression tag	UNP P0DTC2
A	1226	LYS	-	expression tag	UNP P0DTC2
A	1227	ASP	-	expression tag	UNP P0DTC2
A	1228	GLY	-	expression tag	UNP P0DTC2
A	1229	GLU	-	expression tag	UNP P0DTC2
A	1230	TRP	-	expression tag	UNP P0DTC2
A	1231	VAL	-	expression tag	UNP P0DTC2
A	1232	LEU	-	expression tag	UNP P0DTC2
A	1233	LEU	-	expression tag	UNP P0DTC2
A	1234	SER	-	expression tag	UNP P0DTC2
A	1235	THR	-	expression tag	UNP P0DTC2
A	1236	PHE	-	expression tag	UNP P0DTC2
A	1237	LEU	-	expression tag	UNP P0DTC2
A	1238	GLY	-	expression tag	UNP P0DTC2
A	1239	ARG	-	expression tag	UNP P0DTC2
A	1240	SER	-	expression tag	UNP P0DTC2
A	1241	LEU	-	expression tag	UNP P0DTC2
A	1242	GLU	-	expression tag	UNP P0DTC2
A	1243	VAL	-	expression tag	UNP P0DTC2
A	1244	LEU	-	expression tag	UNP P0DTC2
A	1245	PHE	-	expression tag	UNP P0DTC2
A	1246	GLN	-	expression tag	UNP P0DTC2
A	1247	GLY	-	expression tag	UNP P0DTC2
A	1248	PRO	-	expression tag	UNP P0DTC2
A	1249	GLY	-	expression tag	UNP P0DTC2
A	1250	HIS	-	expression tag	UNP P0DTC2
A	1251	HIS	-	expression tag	UNP P0DTC2
A	1252	HIS	-	expression tag	UNP P0DTC2
A	1253	HIS	-	expression tag	UNP P0DTC2
A	1254	HIS	-	expression tag	UNP P0DTC2
A	1255	HIS	-	expression tag	UNP P0DTC2
A	1256	HIS	-	expression tag	UNP P0DTC2
A	1257	HIS	-	expression tag	UNP P0DTC2
A	1258	SER	-	expression tag	UNP P0DTC2

*Continued on next page...*

*Continued from previous page...*

Chain	Residue	Modelled	Actual	Comment	Reference
A	1259	ALA	-	expression tag	UNP P0DTC2
A	1260	TRP	-	expression tag	UNP P0DTC2
A	1261	SER	-	expression tag	UNP P0DTC2
A	1262	HIS	-	expression tag	UNP P0DTC2
A	1263	PRO	-	expression tag	UNP P0DTC2
A	1264	GLN	-	expression tag	UNP P0DTC2
A	1265	PHE	-	expression tag	UNP P0DTC2
A	1266	GLU	-	expression tag	UNP P0DTC2
A	1267	LYS	-	expression tag	UNP P0DTC2
A	1268	GLY	-	expression tag	UNP P0DTC2
A	1269	GLY	-	expression tag	UNP P0DTC2
A	1270	GLY	-	expression tag	UNP P0DTC2
A	1271	SER	-	expression tag	UNP P0DTC2
A	1272	GLY	-	expression tag	UNP P0DTC2
A	1273	GLY	-	expression tag	UNP P0DTC2
A	1274	GLY	-	expression tag	UNP P0DTC2
A	1275	GLY	-	expression tag	UNP P0DTC2
A	1276	SER	-	expression tag	UNP P0DTC2
A	1277	GLY	-	expression tag	UNP P0DTC2
A	1278	GLY	-	expression tag	UNP P0DTC2
A	1279	SER	-	expression tag	UNP P0DTC2
A	1280	ALA	-	expression tag	UNP P0DTC2
A	1281	TRP	-	expression tag	UNP P0DTC2
A	1282	SER	-	expression tag	UNP P0DTC2
A	1283	HIS	-	expression tag	UNP P0DTC2
A	1284	PRO	-	expression tag	UNP P0DTC2
A	1285	GLN	-	expression tag	UNP P0DTC2
A	1286	PHE	-	expression tag	UNP P0DTC2
A	1287	GLU	-	expression tag	UNP P0DTC2
A	1288	LYS	-	expression tag	UNP P0DTC2

- Molecule 2 is a protein called BD-821H.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	120	Total	C	N	O	S	0	0
			933	599	153	177	4		

- Molecule 3 is a protein called BD-821L.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	108	Total	C	N	O	S	0	0
			840	530	143	164	3		

- Molecule 4 is a protein called BD-771H.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	H	129	Total	C	N	O	S	0	0
			1014	649	169	193	3		

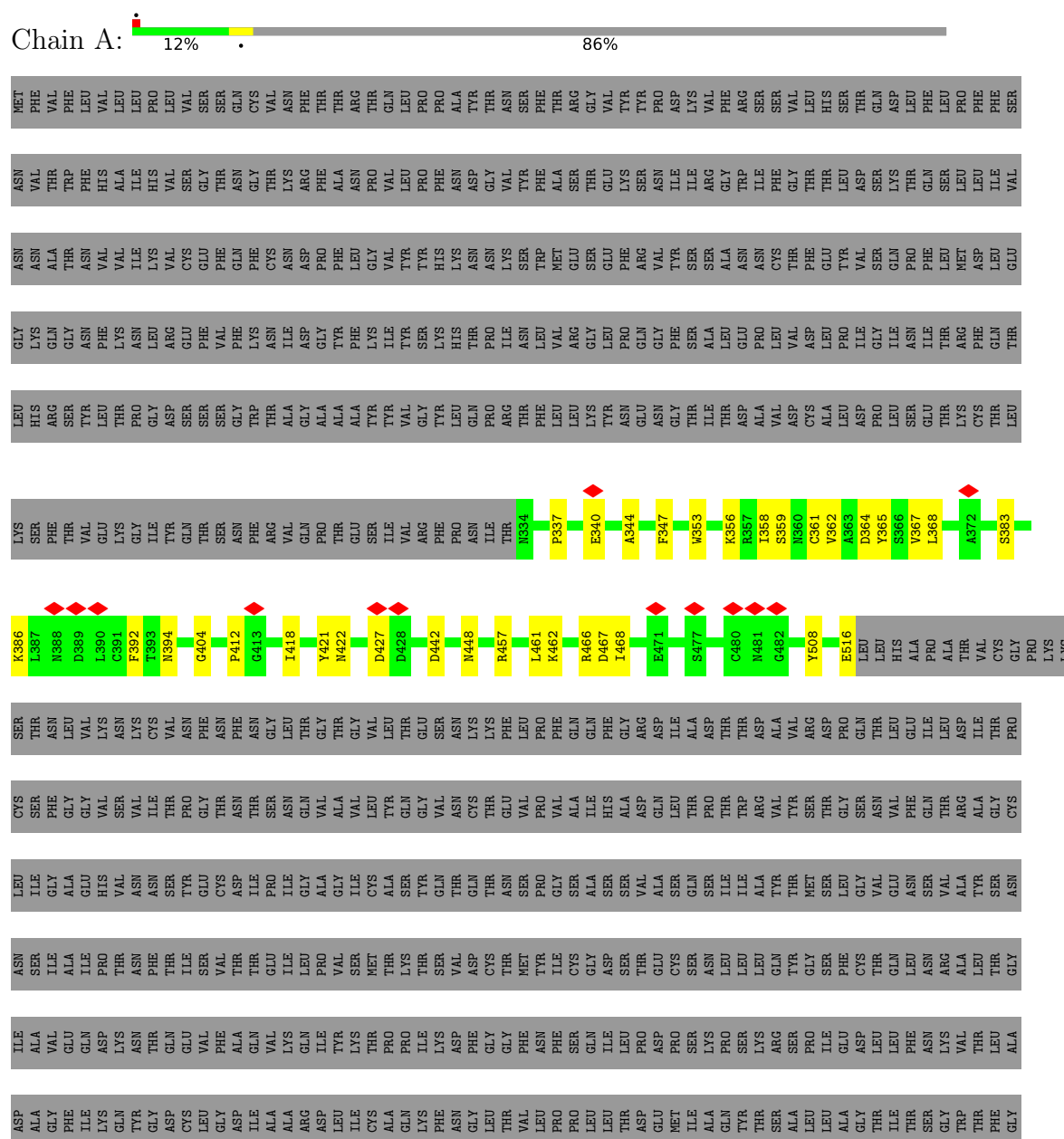
- Molecule 5 is a protein called BD-771L.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	108	Total	C	N	O	S	0	0
			820	518	137	162	3		

### 3 Residue-property plots

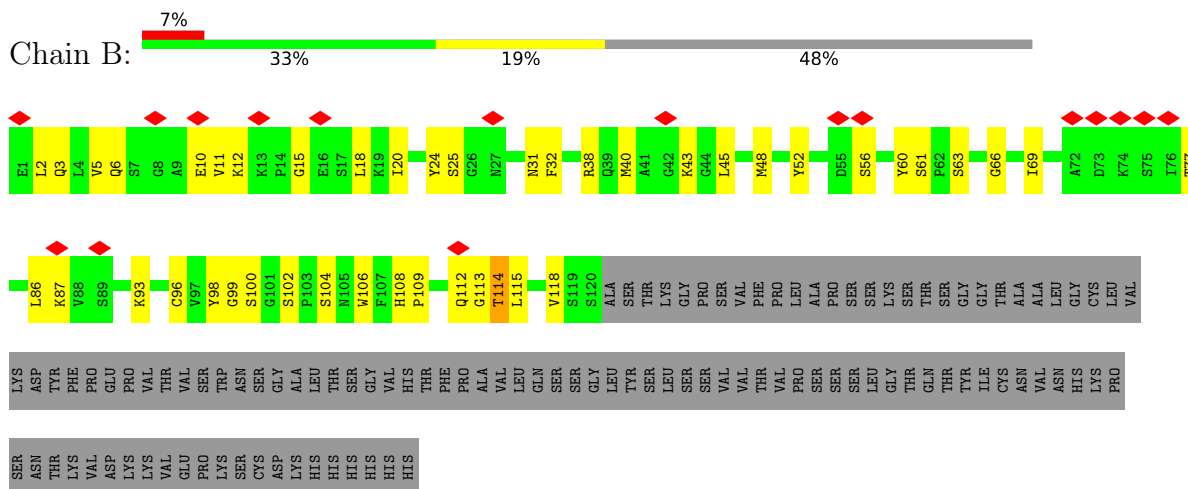
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion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

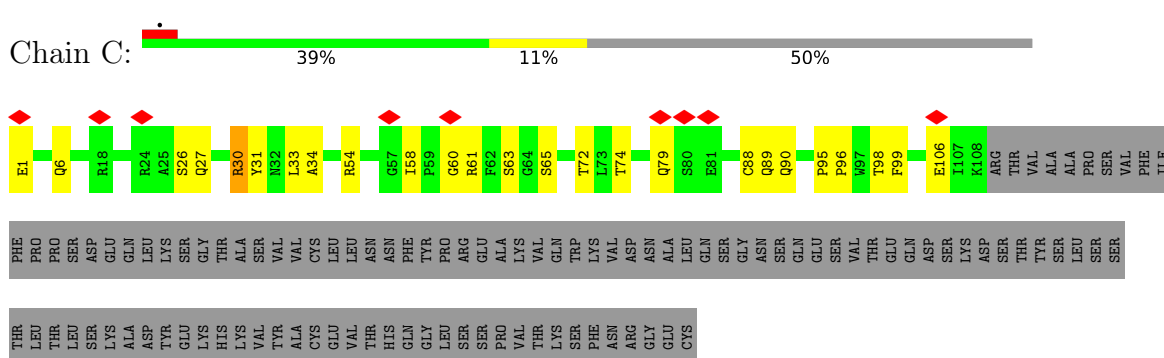


HIS	ALA	ILE	ALA	GLN	GLN	ASP	ALA
HIS	ASN	ILE	GLU	GLN	LEU	VAL	GLY
HIS	LEU	VAL	LYS	ILE	ASN	VAL	PRO
HIS	ASN	ASN	LYS	ARG	GLN	ASN	ALA
HIS	GLU	ASN	PHE	ALA	ASN	ASN	GLN
HIS	SER	THR	THR	THR	ALA	ALA	ILE
HIS	LEU	VAL	THR	GLU	GLU	GLN	PRO
SER	ILE	TYR	ALA	ALA	ILE	ALA	PHE
ALA	ASP	ASP	PRO	ARG	ARG	LEU	PRO
LEU	LEU	PRO	ALA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

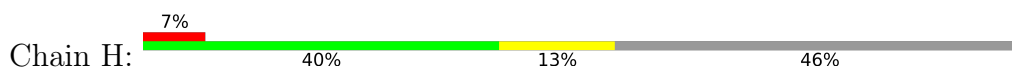
- Molecule 2: BD-821H



- Molecule 3: BD-821L

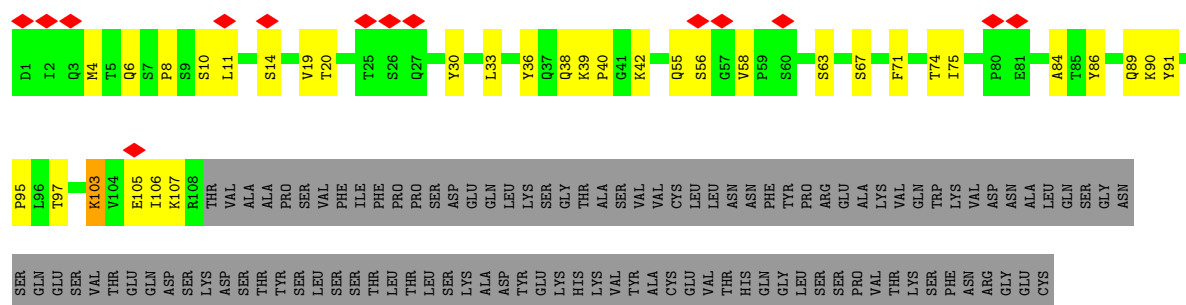
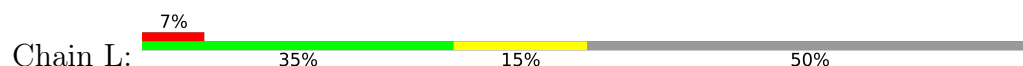


- Molecule 4: BD-771H





- Molecule 5: BD-771L



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	425986	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	59	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	6.974	Depositor
Minimum map value	-4.766	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.039	Depositor
Recommended contour level	0.518	Depositor
Map size ( $\text{\AA}$ )	436.0, 436.0, 436.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.09, 1.09, 1.09	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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	0.32	0/1507	0.45	0/2049
2	B	0.37	0/961	0.58	0/1306
3	C	0.35	0/862	0.54	0/1174
4	H	0.34	0/1042	0.54	0/1412
5	L	0.36	0/837	0.55	0/1134
All	All	0.34	0/5209	0.52	0/7075

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	2
4	H	0	1
All	All	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	114	THR	Peptide
2	B	31	ASN	Peptide
4	H	27	PHE	Peptide

### 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	1465	0	1381	23	0
2	B	933	0	904	29	0
3	C	840	0	808	15	0
4	H	1014	0	960	25	0
5	L	820	0	820	25	0
All	All	5072	0	4873	111	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 11.

All (111) 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)
2:B:6:GLN:NE2	2:B:96:CYS:SG	2.57	0.78
4:H:38:ARG:NH1	4:H:46:GLU:OE1	2.20	0.75
2:B:66:GLY:HA3	2:B:86:LEU:HD11	1.69	0.73
2:B:15:GLY:H	2:B:87:LYS:HG3	1.54	0.72
4:H:54:LYS:HA	4:H:58:GLN:HB2	1.71	0.71
5:L:20:THR:HA	5:L:74:THR:HG22	1.75	0.68
2:B:102:SER:O	2:B:104:SER:N	2.23	0.68
4:H:18:LEU:HD12	4:H:19:ARG:H	1.59	0.67
4:H:105:GLU:HB3	4:H:110:ASP:HB3	1.77	0.67
5:L:6:GLN:NE2	5:L:86:TYR:O	2.16	0.67
2:B:112:GLN:NE2	2:B:113:GLY:O	2.27	0.66
4:H:53:SER:HA	4:H:74:ARG:HH12	1.61	0.66
3:C:6:GLN:NE2	3:C:88:CYS:SG	2.67	0.66
5:L:40:PRO:O	5:L:42:LYS:NZ	2.21	0.66
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.62	0.65
2:B:12:LYS:HD3	2:B:18:LEU:HD11	1.78	0.65
1:A:353:TRP:O	1:A:466:ARG:NH1	2.30	0.64
1:A:367:VAL:HG23	1:A:368:LEU:HD12	1.80	0.63
1:A:421:TYR:OH	4:H:107:ARG:NH1	2.32	0.63
2:B:108:HIS:HB3	2:B:109:PRO:HD3	1.81	0.63
2:B:2:LEU:HG	2:B:3:GLN:H	1.62	0.62
4:H:102:ALA:HB2	4:H:116:TYR:CE2	2.35	0.62
4:H:62:TYR:HB2	4:H:67:LYS:HD2	1.84	0.60
4:H:66:VAL:HG13	4:H:70:PHE:HD2	1.65	0.60
5:L:19:VAL:HB	5:L:75:ILE:HG22	1.84	0.60
1:A:356:LYS:HE3	1:A:358:ILE:HD11	1.84	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:40:MET:HB2	2:B:43:LYS:HB2	1.84	0.59
5:L:63:SER:OG	5:L:74:THR:OG1	2.21	0.58
2:B:93:LYS:NZ	2:B:114:THR:O	2.33	0.58
5:L:8:PRO:HG2	5:L:11:LEU:HD11	1.85	0.58
5:L:14:SER:H	5:L:107:LYS:HE2	1.70	0.57
2:B:98:TYR:HB3	2:B:109:PRO:HD2	1.86	0.56
2:B:32:PHE:HE1	2:B:98:TYR:HE1	1.55	0.54
5:L:39:LYS:HB3	5:L:42:LYS:HZ2	1.71	0.54
3:C:89:GLN:HG2	3:C:90:GLN:O	2.07	0.54
2:B:24:TYR:CD2	2:B:77:THR:HB	2.41	0.54
3:C:61:ARG:NH2	3:C:79:GLN:OE1	2.41	0.54
4:H:53:SER:HA	4:H:74:ARG:NH1	2.23	0.53
3:C:33:LEU:HG	3:C:34:ALA:H	1.74	0.53
3:C:106:GLU:N	3:C:106:GLU:OE2	2.41	0.53
3:C:26:SER:OG	3:C:27:GLN:OE1	2.19	0.53
1:A:418:ILE:HA	1:A:422:ASN:HB2	1.91	0.52
4:H:93:THR:OG1	4:H:128:VAL:N	2.42	0.52
1:A:359:SER:OG	1:A:394:ASN:OD1	2.20	0.52
5:L:39:LYS:HG3	5:L:84:ALA:HB2	1.90	0.52
3:C:95:PRO:HB2	3:C:96:PRO:HD3	1.92	0.52
1:A:442:ASP:O	1:A:448:ASN:ND2	2.41	0.52
1:A:353:TRP:CZ2	1:A:466:ARG:HB3	2.44	0.52
1:A:361:CYS:SG	1:A:362:VAL:N	2.84	0.51
5:L:30:TYR:O	5:L:67:SER:OG	2.27	0.51
4:H:6:GLU:OE2	4:H:123:GLY:N	2.39	0.50
4:H:18:LEU:HD12	4:H:19:ARG:N	2.26	0.50
1:A:383:SER:HB3	1:A:386:LYS:HB2	1.93	0.50
2:B:20:ILE:HG23	2:B:115:LEU:HD12	1.93	0.49
3:C:63:SER:OG	3:C:74:THR:OG1	2.29	0.49
4:H:4:LEU:HD23	4:H:24:ALA:HA	1.95	0.49
1:A:457:ARG:HE	1:A:461:LEU:HD22	1.78	0.48
2:B:100:SER:O	2:B:106:TRP:NE1	2.45	0.48
3:C:54:ARG:CZ	3:C:60:GLY:HA2	2.42	0.48
4:H:115:TYR:HB3	5:L:91:TYR:HE1	1.78	0.48
2:B:10:GLU:CD	2:B:11:VAL:H	2.16	0.48
2:B:2:LEU:HB3	2:B:25:SER:CB	2.44	0.48
2:B:38:ARG:HB3	2:B:48:MET:HE3	1.95	0.48
3:C:54:ARG:HB3	3:C:58:ILE:HD11	1.97	0.47
4:H:67:LYS:HD2	4:H:67:LYS:HA	1.73	0.47
2:B:98:TYR:CG	2:B:99:GLY:N	2.83	0.47
2:B:32:PHE:CE1	2:B:98:TYR:HE1	2.32	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:1:GLU:HA	3:C:96:PRO:HG2	1.97	0.47
5:L:33:LEU:HD13	5:L:71:PHE:CD2	2.49	0.47
2:B:15:GLY:N	2:B:87:LYS:HG3	2.28	0.47
2:B:61:SER:O	2:B:63:SER:N	2.44	0.46
1:A:404:GLY:HA2	1:A:508:TYR:CD1	2.51	0.46
2:B:60:TYR:OH	2:B:69:ILE:N	2.42	0.46
3:C:65:SER:HB2	3:C:72:THR:HB	1.97	0.46
5:L:55:GLN:OE1	5:L:56:SER:N	2.48	0.46
5:L:89:GLN:HG2	5:L:90:LYS:O	2.15	0.46
2:B:45:LEU:HD12	3:C:99:PHE:CE2	2.51	0.46
3:C:96:PRO:O	3:C:98:THR:HG23	2.16	0.46
4:H:3:GLN:N	4:H:3:GLN:OE1	2.49	0.46
5:L:10:SER:C	5:L:11:LEU:HD12	2.36	0.45
1:A:418:ILE:HD12	1:A:418:ILE:H	1.82	0.45
5:L:55:GLN:O	5:L:58:VAL:HG12	2.16	0.45
4:H:62:TYR:HE1	4:H:72:ILE:HG13	1.81	0.45
4:H:115:TYR:HB3	5:L:91:TYR:CE1	2.52	0.45
1:A:344:ALA:HB3	1:A:347:PHE:HE1	1.81	0.45
5:L:33:LEU:HD22	5:L:71:PHE:HD2	1.80	0.45
2:B:3:GLN:OE1	2:B:5:VAL:HG23	2.18	0.44
1:A:421:TYR:CD1	1:A:457:ARG:HB3	2.53	0.43
1:A:421:TYR:HA	1:A:461:LEU:HD23	2.00	0.43
1:A:462:LYS:HE2	1:A:462:LYS:HB2	1.81	0.43
4:H:36:TRP:O	4:H:48:VAL:HG12	2.19	0.43
5:L:105:GLU:HG2	5:L:106:ILE:H	1.84	0.43
1:A:467:ASP:O	1:A:468:ILE:HD13	2.18	0.43
3:C:30:ARG:HG2	3:C:31:TYR:N	2.34	0.43
4:H:54:LYS:HD2	4:H:54:LYS:O	2.18	0.43
2:B:6:GLN:HB3	2:B:115:LEU:HD11	2.00	0.42
1:A:364:ASP:OD1	1:A:365:TYR:N	2.52	0.42
2:B:52:TYR:O	2:B:56:SER:HA	2.19	0.42
5:L:95:PRO:HG2	5:L:97:THR:HG23	2.01	0.42
4:H:17:SER:OG	4:H:86:HIS:O	2.37	0.42
1:A:337:PRO:O	1:A:340:GLU:HG3	2.19	0.42
4:H:116:TYR:HD2	5:L:91:TYR:CE1	2.38	0.42
4:H:117:PHE:N	5:L:36:TYR:OH	2.44	0.42
5:L:38:GLN:NE2	5:L:42:LYS:O	2.53	0.42
2:B:10:GLU:OE1	2:B:11:VAL:HG12	2.20	0.41
5:L:14:SER:N	5:L:107:LYS:HE2	2.34	0.41
1:A:392:PHE:HB3	1:A:516:GLU:HB2	2.03	0.41
1:A:412:PRO:HB2	1:A:427:ASP:HA	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:35:ASN:ND2	4:H:117:PHE:HE1	2.18	0.41
2:B:11:VAL:HA	2:B:118:VAL:HB	2.03	0.40
5:L:10:SER:HA	5:L:103:LYS:HE3	2.04	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	181/1285 (14%)	169 (93%)	12 (7%)	0	100	100
2	B	118/231 (51%)	90 (76%)	28 (24%)	0	100	100
3	C	106/215 (49%)	91 (86%)	15 (14%)	0	100	100
4	H	127/241 (53%)	110 (87%)	17 (13%)	0	100	100
5	L	106/214 (50%)	96 (91%)	10 (9%)	0	100	100
All	All	638/2186 (29%)	556 (87%)	82 (13%)	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	159/1112 (14%)	159 (100%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	103/200 (52%)	103 (100%)	0	100	100
3	C	91/187 (49%)	90 (99%)	1 (1%)	70	81
4	H	105/203 (52%)	104 (99%)	1 (1%)	73	83
5	L	92/187 (49%)	90 (98%)	2 (2%)	47	68
All	All	550/1889 (29%)	546 (99%)	4 (1%)	80	88

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	30	ARG
4	H	54	LYS
5	L	4	MET
5	L	103	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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](#)

There are no ligands in this entry.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

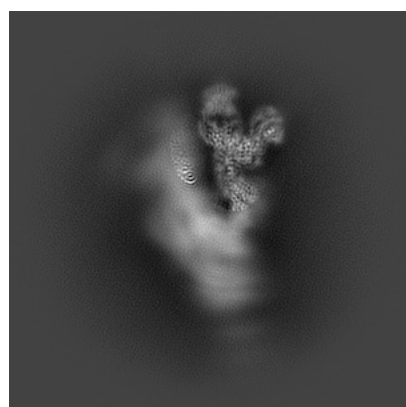
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31378. These allow visual inspection of the internal detail of the map and identification of artifacts.

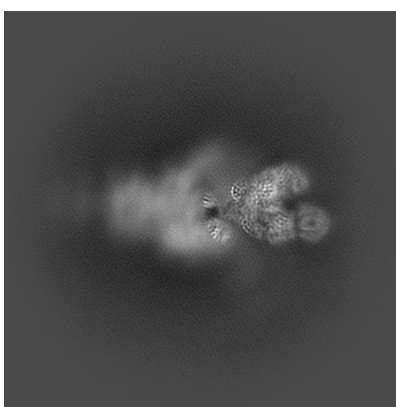
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

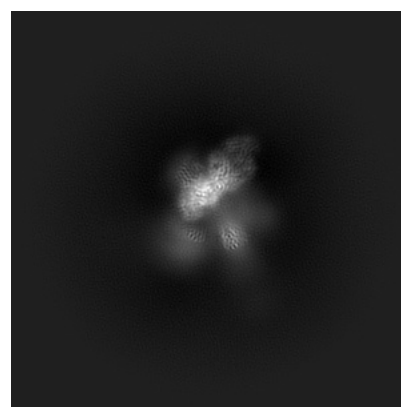
#### 6.1.1 Primary map



X



Y

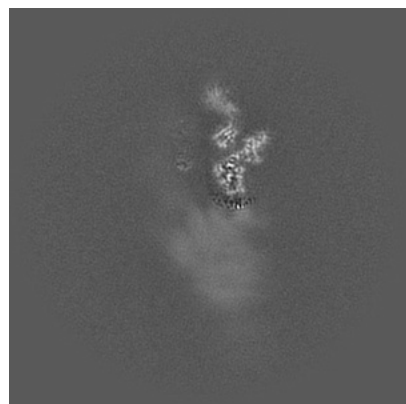


Z

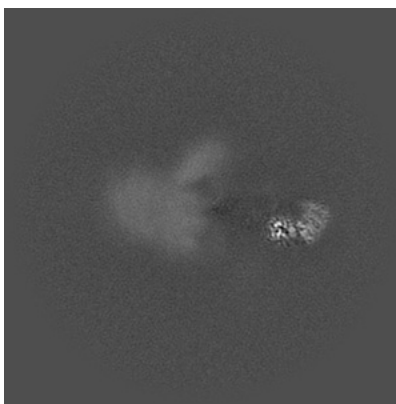
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

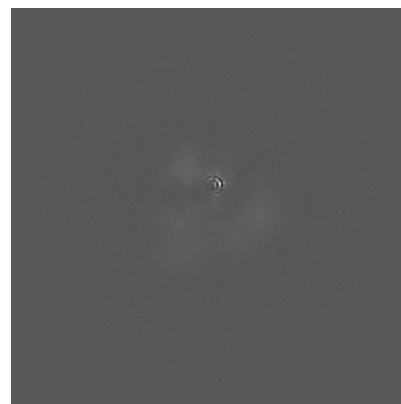
#### 6.2.1 Primary map



X Index: 200



Y Index: 200

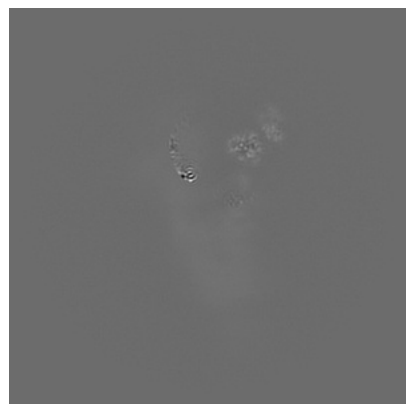


Z Index: 200

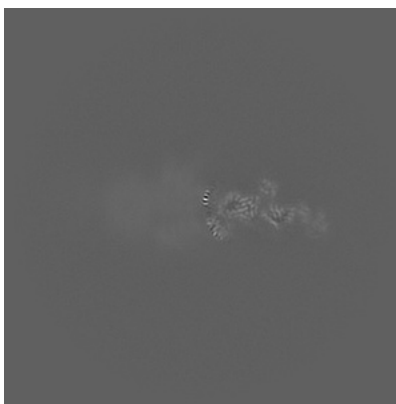
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

### 6.3.1 Primary map



X Index: 218



Y Index: 223

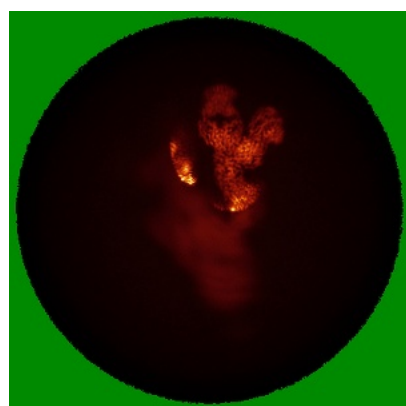


Z Index: 231

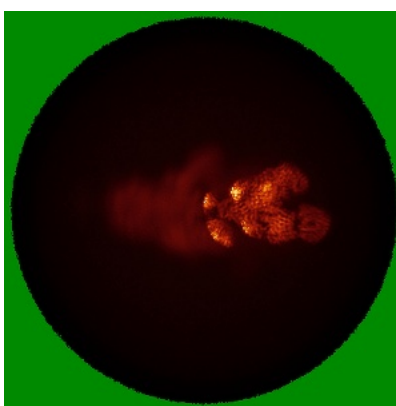
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

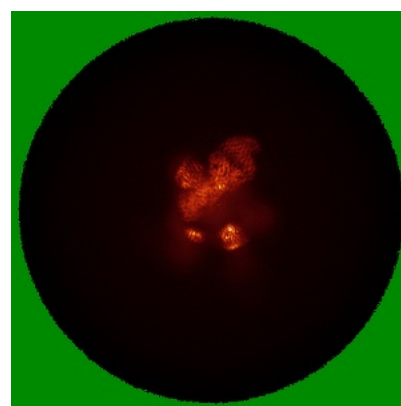
### 6.4.1 Primary map



X



Y

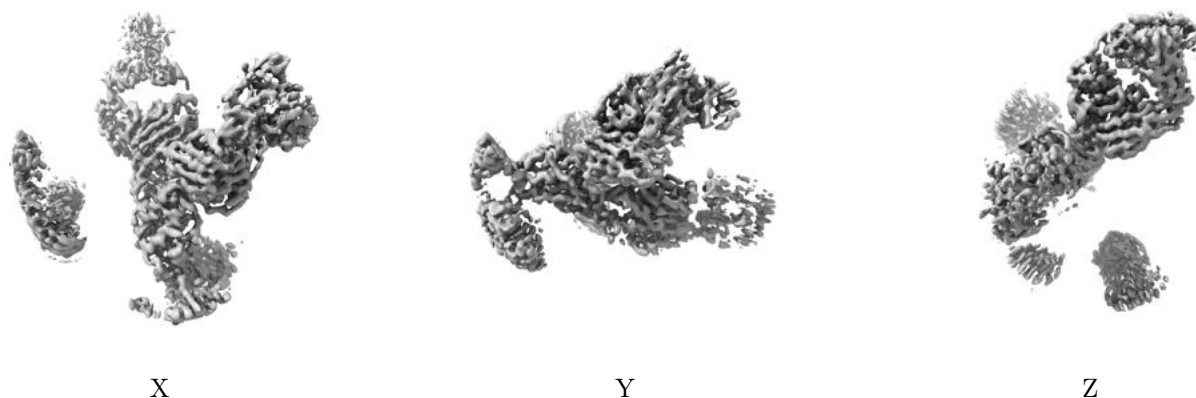


Z

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



The images above show the 3D surface view of the map at the recommended contour level 0.518. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

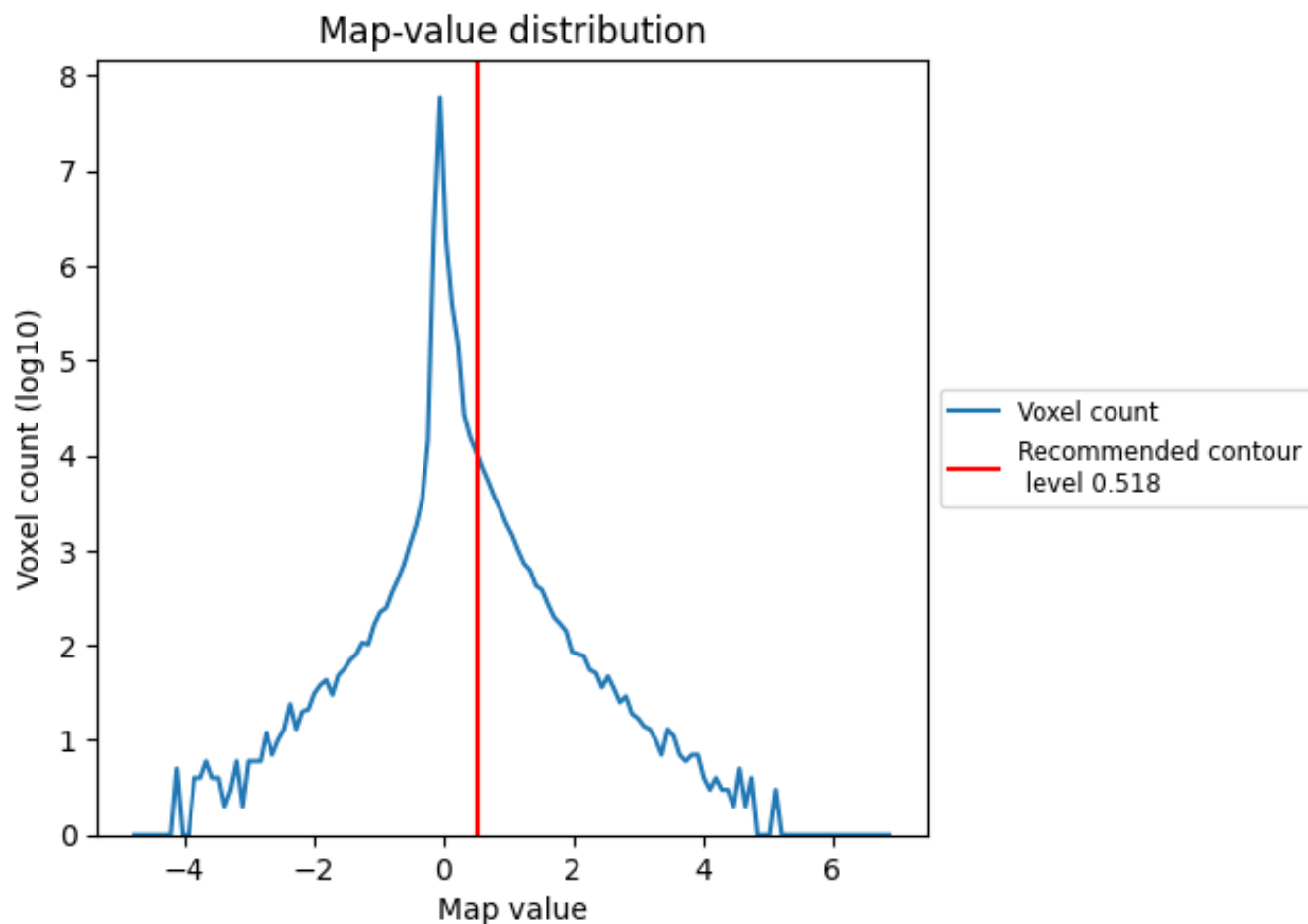
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

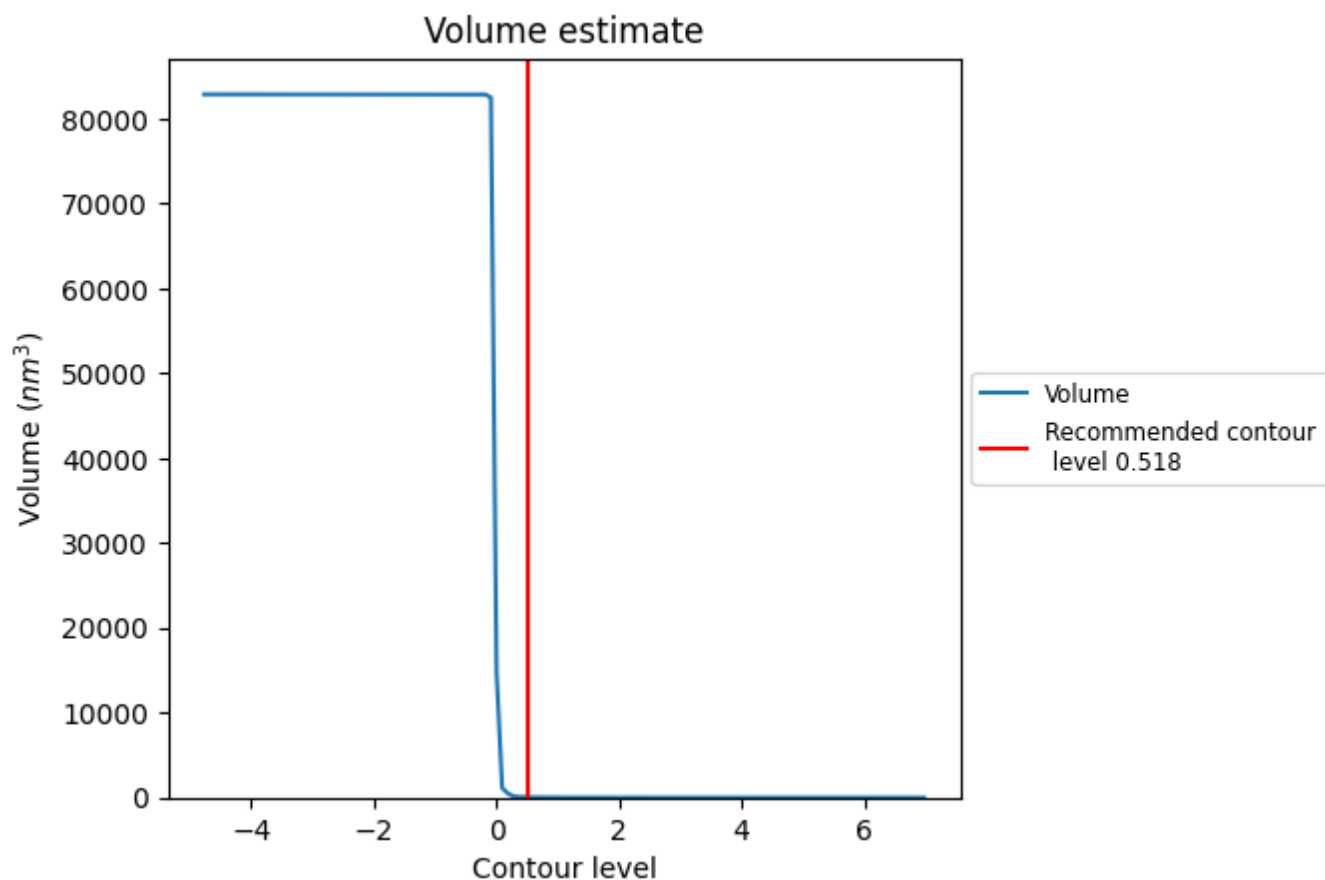
This section contains the results of statistical analysis of the map.

### 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.

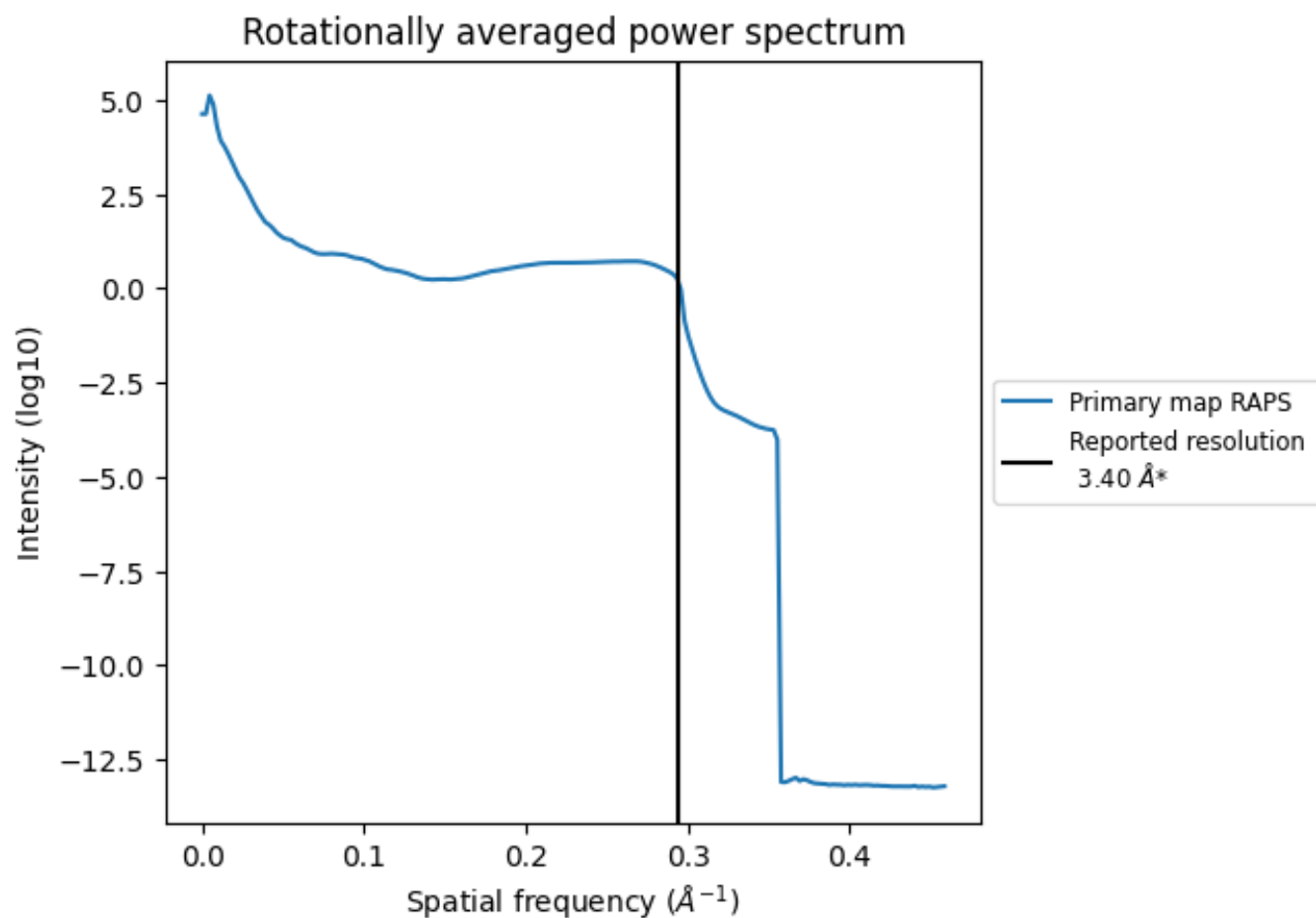
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 47  $\text{nm}^3$ ; this corresponds to an approximate mass of 43 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 ⓘ



\*Reported resolution corresponds to spatial frequency of 0.294 Å<sup>-1</sup>

## 8 Fourier-Shell correlation ⓘ

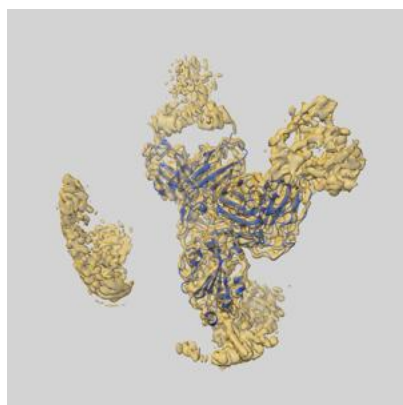
This section was not generated. No FSC curve or half-maps provided.



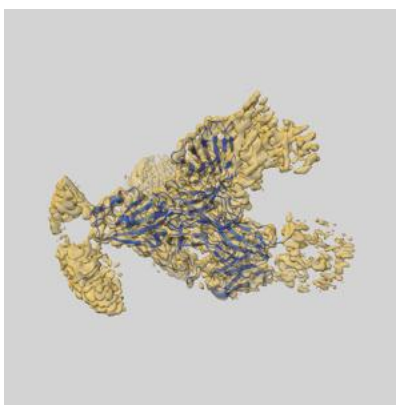
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-31378 and PDB model 7EY5. Per-residue inclusion information can be found in section [3](#) on page [7](#).

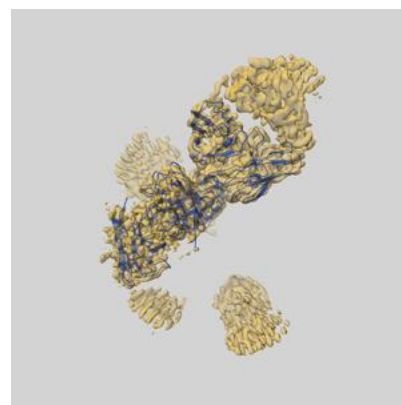
### 9.1 Map-model overlay [i](#)



X



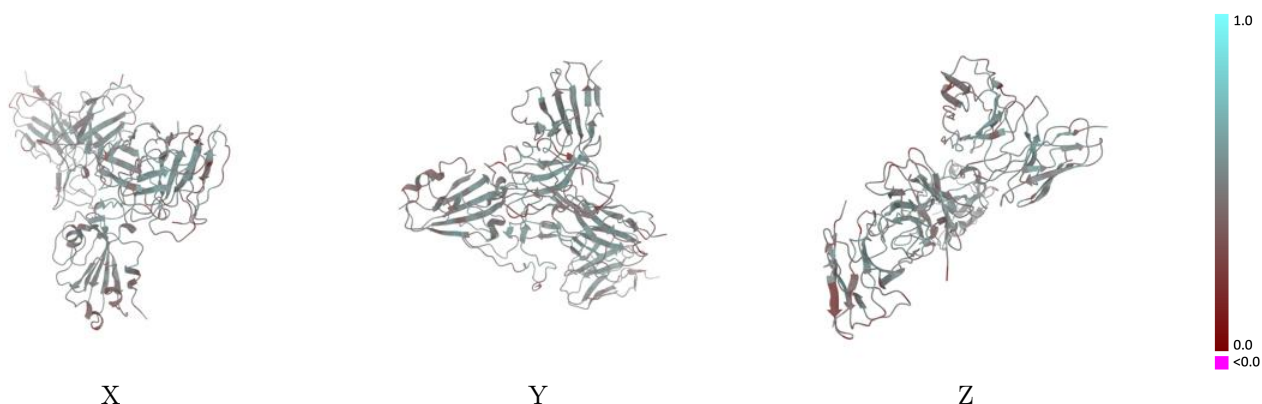
Y



Z

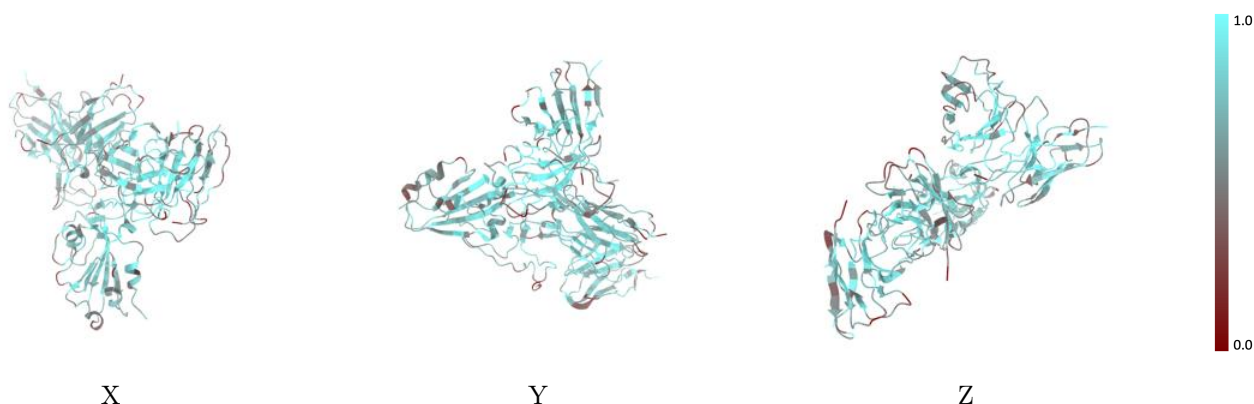
The images above show the 3D surface view of the map at the recommended contour level 0.518 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 9.2 Q-score mapped to coordinate model [i](#)



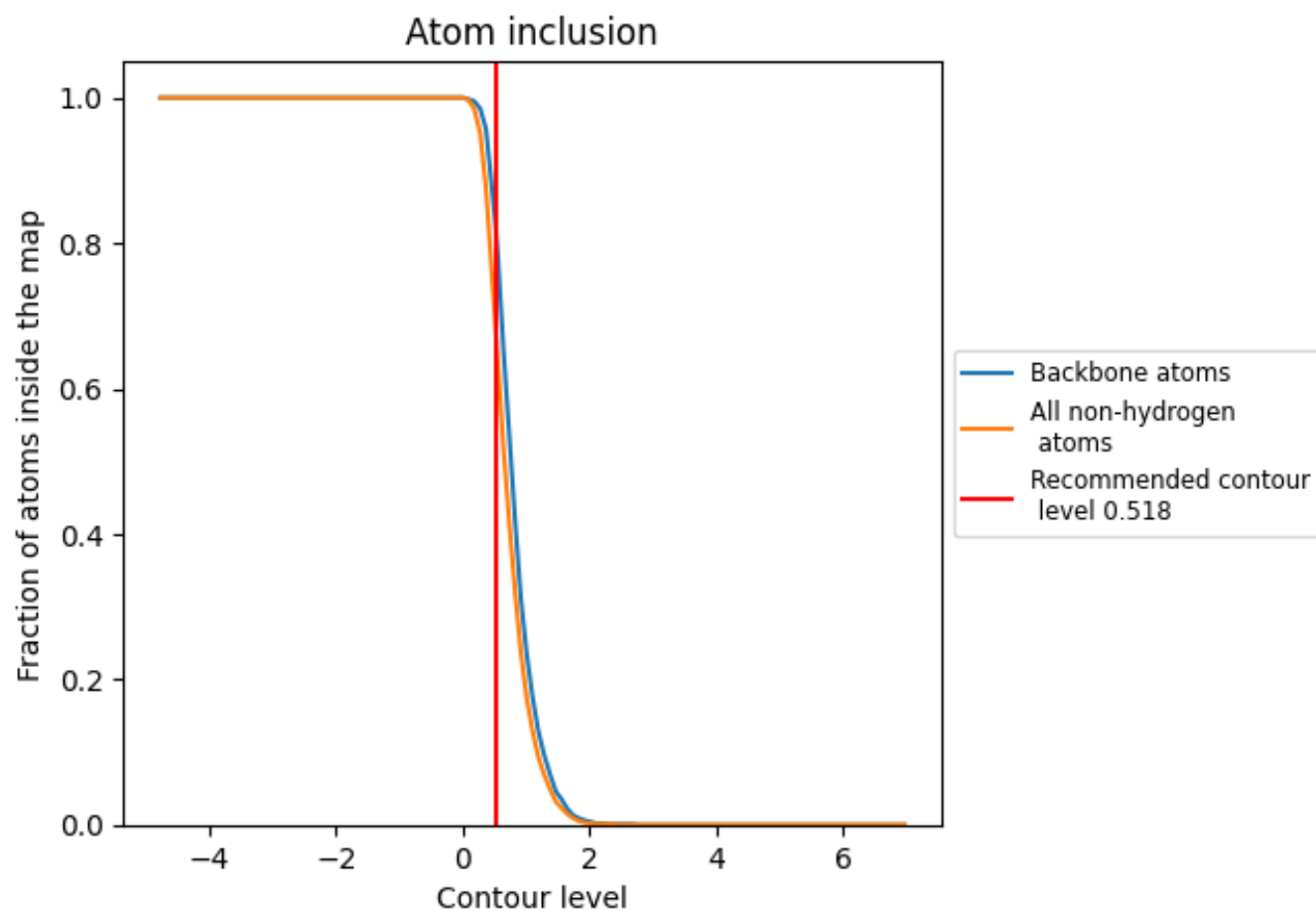
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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](#)



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 (0.518).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 69% 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 (0.518) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6890	<div></div> 0.4850
A	<div></div> 0.7020	<div></div> 0.4890
B	<div></div> 0.6890	<div></div> 0.4730
C	<div></div> 0.7170	<div></div> 0.5010
H	<div></div> 0.6570	<div></div> 0.4890
L	<div></div> 0.6780	<div></div> 0.4710

