



# wwPDB EM Validation Summary Report ⓘ

Oct 6, 2024 – 03:17 AM JST

PDB ID : 7F2O  
EMDB ID : EMD-31429  
Title : Cryo-EM structure of the type 2 bradykinin receptor in complex with the bradykinin and an Gq protein  
Authors : Yin, Y.; Jiang, Y.  
Deposited on : 2021-06-11  
Resolution : 2.90 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](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>.

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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

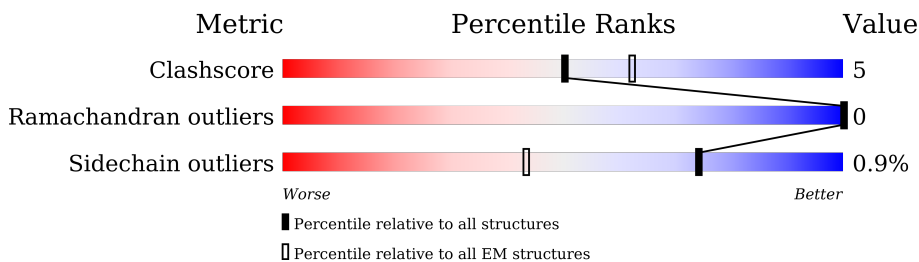
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 2.90 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	361	 53% 11% 36%
2	B	377	 78% 12% 10%
3	D	9	 56% 44%
4	R	595	 39% 9% 52%
5	S	248	 85% 8% 6%
6	Y	71	 69% 28%

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9004 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 G subunit q (Gi1-Gq chimeric).

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	230	Total	C	N	O	S	0	0
			1878	1186	334	350	8		

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	341	Total	C	N	O	S	0	0
			2605	1607	469	508	21		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-10	MET	-	initiating methionine	UNP P54311
B	-9	HIS	-	expression tag	UNP P54311
B	-8	HIS	-	expression tag	UNP P54311
B	-7	HIS	-	expression tag	UNP P54311
B	-6	HIS	-	expression tag	UNP P54311
B	-5	HIS	-	expression tag	UNP P54311
B	-4	HIS	-	expression tag	UNP P54311
B	-3	GLY	-	expression tag	UNP P54311
B	-2	SER	-	expression tag	UNP P54311
B	-1	LEU	-	expression tag	UNP P54311
B	0	LEU	-	expression tag	UNP P54311
B	1	GLN	-	expression tag	UNP P54311
B	341	GLY	-	expression tag	UNP P54311
B	342	SER	-	expression tag	UNP P54311
B	343	SER	-	expression tag	UNP P54311
B	344	GLY	-	expression tag	UNP P54311
B	345	GLY	-	expression tag	UNP P54311
B	346	GLY	-	expression tag	UNP P54311
B	347	GLY	-	expression tag	UNP P54311
B	348	SER	-	expression tag	UNP P54311

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Chain	Residue	Modelled	Actual	Comment	Reference
B	349	GLY	-	expression tag	UNP P54311
B	350	GLY	-	expression tag	UNP P54311
B	351	GLY	-	expression tag	UNP P54311
B	352	GLY	-	expression tag	UNP P54311
B	353	SER	-	expression tag	UNP P54311
B	354	SER	-	expression tag	UNP P54311
B	355	GLY	-	expression tag	UNP P54311
B	356	VAL	-	expression tag	UNP P54311
B	357	SER	-	expression tag	UNP P54311
B	358	GLY	-	expression tag	UNP P54311
B	359	TRP	-	expression tag	UNP P54311
B	360	ARG	-	expression tag	UNP P54311
B	361	LEU	-	expression tag	UNP P54311
B	362	PHE	-	expression tag	UNP P54311
B	363	LYS	-	expression tag	UNP P54311
B	364	LYS	-	expression tag	UNP P54311
B	365	ILE	-	expression tag	UNP P54311
B	366	SER	-	expression tag	UNP P54311

- Molecule 3 is a protein called ARG-PRO-PRO-GLY-PHE-SER-PRO-PHE-ARG.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	D	9	Total	C	N	O	0	0
			76	50	15	11		

- Molecule 4 is a protein called B2 bradykinin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	R	287	Total	C	N	O	S	0	0
			2308	1524	371	391	22		

There are 265 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-66	ALA	-	expression tag	UNP P30411
R	-65	ASP	-	expression tag	UNP P30411
R	-64	LEU	-	expression tag	UNP P30411
R	-63	GLU	-	expression tag	UNP P30411
R	-62	ASP	-	expression tag	UNP P30411
R	-61	ASN	-	expression tag	UNP P30411
R	-60	TRP	-	expression tag	UNP P30411
R	-59	GLU	-	expression tag	UNP P30411

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-58	THR	-	expression tag	UNP P30411
R	-57	LEU	-	expression tag	UNP P30411
R	-56	ASN	-	expression tag	UNP P30411
R	-55	ASP	-	expression tag	UNP P30411
R	-54	ASN	-	expression tag	UNP P30411
R	-53	LEU	-	expression tag	UNP P30411
R	-52	LYS	-	expression tag	UNP P30411
R	-51	VAL	-	expression tag	UNP P30411
R	-50	ILE	-	expression tag	UNP P30411
R	-49	GLU	-	expression tag	UNP P30411
R	-48	LYS	-	expression tag	UNP P30411
R	-47	ALA	-	expression tag	UNP P30411
R	-46	ASP	-	expression tag	UNP P30411
R	-45	ASN	-	expression tag	UNP P30411
R	-44	ALA	-	expression tag	UNP P30411
R	-43	ALA	-	expression tag	UNP P30411
R	-42	GLN	-	expression tag	UNP P30411
R	-41	VAL	-	expression tag	UNP P30411
R	-40	LYS	-	expression tag	UNP P30411
R	-39	ASP	-	expression tag	UNP P30411
R	-38	ALA	-	expression tag	UNP P30411
R	-37	LEU	-	expression tag	UNP P30411
R	-36	THR	-	expression tag	UNP P30411
R	-35	LYS	-	expression tag	UNP P30411
R	-34	MET	-	expression tag	UNP P30411
R	-33	ARG	-	expression tag	UNP P30411
R	-32	ALA	-	expression tag	UNP P30411
R	-31	ALA	-	expression tag	UNP P30411
R	-30	ALA	-	expression tag	UNP P30411
R	-29	LEU	-	expression tag	UNP P30411
R	-28	ASP	-	expression tag	UNP P30411
R	-27	ALA	-	expression tag	UNP P30411
R	-26	GLN	-	expression tag	UNP P30411
R	-25	LYS	-	expression tag	UNP P30411
R	-24	ALA	-	expression tag	UNP P30411
R	-23	THR	-	expression tag	UNP P30411
R	-22	PRO	-	expression tag	UNP P30411
R	-21	PRO	-	expression tag	UNP P30411
R	-20	LYS	-	expression tag	UNP P30411
R	-19	LEU	-	expression tag	UNP P30411
R	-18	GLU	-	expression tag	UNP P30411
R	-17	ASP	-	expression tag	UNP P30411

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-16	LYS	-	expression tag	UNP P30411
R	-15	SER	-	expression tag	UNP P30411
R	-14	PRO	-	expression tag	UNP P30411
R	-13	ASP	-	expression tag	UNP P30411
R	-12	SER	-	expression tag	UNP P30411
R	-11	PRO	-	expression tag	UNP P30411
R	-10	GLU	-	expression tag	UNP P30411
R	-9	MET	-	expression tag	UNP P30411
R	-8	LYS	-	expression tag	UNP P30411
R	-7	ASP	-	expression tag	UNP P30411
R	-6	PHE	-	expression tag	UNP P30411
R	-5	ARG	-	expression tag	UNP P30411
R	-4	HIS	-	expression tag	UNP P30411
R	-3	GLY	-	expression tag	UNP P30411
R	-2	PHE	-	expression tag	UNP P30411
R	-1	ASP	-	expression tag	UNP P30411
R	0	ILE	-	expression tag	UNP P30411
R	1	LEU	-	expression tag	UNP P30411
R	2	VAL	-	expression tag	UNP P30411
R	3	GLY	-	expression tag	UNP P30411
R	4	GLN	-	expression tag	UNP P30411
R	5	ILE	-	expression tag	UNP P30411
R	6	ASP	-	expression tag	UNP P30411
R	7	ASP	-	expression tag	UNP P30411
R	8	ALA	-	expression tag	UNP P30411
R	9	LEU	-	expression tag	UNP P30411
R	10	LYS	-	expression tag	UNP P30411
R	11	LEU	-	expression tag	UNP P30411
R	12	ALA	-	expression tag	UNP P30411
R	13	ASN	-	expression tag	UNP P30411
R	14	GLU	-	expression tag	UNP P30411
R	15	GLY	-	expression tag	UNP P30411
R	16	LYS	-	expression tag	UNP P30411
R	17	VAL	-	expression tag	UNP P30411
R	18	LYS	-	expression tag	UNP P30411
R	19	GLU	-	expression tag	UNP P30411
R	20	ALA	-	expression tag	UNP P30411
R	21	GLN	-	expression tag	UNP P30411
R	22	ALA	-	expression tag	UNP P30411
R	23	ALA	-	expression tag	UNP P30411
R	24	ALA	-	expression tag	UNP P30411
R	25	GLU	-	expression tag	UNP P30411

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Chain	Residue	Modelled	Actual	Comment	Reference
R	26	GLN	-	expression tag	UNP P30411
R	27	LEU	-	expression tag	UNP P30411
R	28	LYS	-	expression tag	UNP P30411
R	29	THR	-	expression tag	UNP P30411
R	30	THR	-	expression tag	UNP P30411
R	31	ARG	-	expression tag	UNP P30411
R	32	ASN	-	expression tag	UNP P30411
R	33	ALA	-	expression tag	UNP P30411
R	34	TYR	-	expression tag	UNP P30411
R	35	ILE	-	expression tag	UNP P30411
R	36	GLN	-	expression tag	UNP P30411
R	37	LYS	-	expression tag	UNP P30411
R	38	TYR	-	expression tag	UNP P30411
R	39	LEU	-	expression tag	UNP P30411
R	146	TRP	CYS	engineered mutation	UNP P30411
R	371	VAL	-	expression tag	UNP P30411
R	372	PHE	-	expression tag	UNP P30411
R	373	THR	-	expression tag	UNP P30411
R	374	LEU	-	expression tag	UNP P30411
R	375	GLU	-	expression tag	UNP P30411
R	376	ASP	-	expression tag	UNP P30411
R	377	PHE	-	expression tag	UNP P30411
R	378	VAL	-	expression tag	UNP P30411
R	379	GLY	-	expression tag	UNP P30411
R	380	ASP	-	expression tag	UNP P30411
R	381	TRP	-	expression tag	UNP P30411
R	382	GLU	-	expression tag	UNP P30411
R	383	GLN	-	expression tag	UNP P30411
R	384	THR	-	expression tag	UNP P30411
R	385	ALA	-	expression tag	UNP P30411
R	386	ALA	-	expression tag	UNP P30411
R	387	TYR	-	expression tag	UNP P30411
R	388	ASN	-	expression tag	UNP P30411
R	389	LEU	-	expression tag	UNP P30411
R	390	ASP	-	expression tag	UNP P30411
R	391	GLN	-	expression tag	UNP P30411
R	392	VAL	-	expression tag	UNP P30411
R	393	LEU	-	expression tag	UNP P30411
R	394	GLU	-	expression tag	UNP P30411
R	395	GLN	-	expression tag	UNP P30411
R	396	GLY	-	expression tag	UNP P30411
R	397	GLY	-	expression tag	UNP P30411

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Chain	Residue	Modelled	Actual	Comment	Reference
R	398	VAL	-	expression tag	UNP P30411
R	399	SER	-	expression tag	UNP P30411
R	400	SER	-	expression tag	UNP P30411
R	401	LEU	-	expression tag	UNP P30411
R	402	LEU	-	expression tag	UNP P30411
R	403	GLN	-	expression tag	UNP P30411
R	404	ASN	-	expression tag	UNP P30411
R	405	LEU	-	expression tag	UNP P30411
R	406	ALA	-	expression tag	UNP P30411
R	407	VAL	-	expression tag	UNP P30411
R	408	SER	-	expression tag	UNP P30411
R	409	VAL	-	expression tag	UNP P30411
R	410	THR	-	expression tag	UNP P30411
R	411	PRO	-	expression tag	UNP P30411
R	412	ILE	-	expression tag	UNP P30411
R	413	GLN	-	expression tag	UNP P30411
R	414	ARG	-	expression tag	UNP P30411
R	415	ILE	-	expression tag	UNP P30411
R	416	VAL	-	expression tag	UNP P30411
R	417	ARG	-	expression tag	UNP P30411
R	418	SER	-	expression tag	UNP P30411
R	419	GLY	-	expression tag	UNP P30411
R	420	GLU	-	expression tag	UNP P30411
R	421	ASN	-	expression tag	UNP P30411
R	422	ALA	-	expression tag	UNP P30411
R	423	LEU	-	expression tag	UNP P30411
R	424	LYS	-	expression tag	UNP P30411
R	425	ILE	-	expression tag	UNP P30411
R	426	ASP	-	expression tag	UNP P30411
R	427	ILE	-	expression tag	UNP P30411
R	428	HIS	-	expression tag	UNP P30411
R	429	VAL	-	expression tag	UNP P30411
R	430	ILE	-	expression tag	UNP P30411
R	431	ILE	-	expression tag	UNP P30411
R	432	PRO	-	expression tag	UNP P30411
R	433	TYR	-	expression tag	UNP P30411
R	434	GLU	-	expression tag	UNP P30411
R	435	GLY	-	expression tag	UNP P30411
R	436	LEU	-	expression tag	UNP P30411
R	437	SER	-	expression tag	UNP P30411
R	438	ALA	-	expression tag	UNP P30411
R	439	ASP	-	expression tag	UNP P30411

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Chain	Residue	Modelled	Actual	Comment	Reference
R	440	GLN	-	expression tag	UNP P30411
R	441	MET	-	expression tag	UNP P30411
R	442	ALA	-	expression tag	UNP P30411
R	443	GLN	-	expression tag	UNP P30411
R	444	ILE	-	expression tag	UNP P30411
R	445	GLU	-	expression tag	UNP P30411
R	446	GLU	-	expression tag	UNP P30411
R	447	VAL	-	expression tag	UNP P30411
R	448	PHE	-	expression tag	UNP P30411
R	449	LYS	-	expression tag	UNP P30411
R	450	VAL	-	expression tag	UNP P30411
R	451	VAL	-	expression tag	UNP P30411
R	452	TYR	-	expression tag	UNP P30411
R	453	PRO	-	expression tag	UNP P30411
R	454	VAL	-	expression tag	UNP P30411
R	455	ASP	-	expression tag	UNP P30411
R	456	ASP	-	expression tag	UNP P30411
R	457	HIS	-	expression tag	UNP P30411
R	458	HIS	-	expression tag	UNP P30411
R	459	PHE	-	expression tag	UNP P30411
R	460	LYS	-	expression tag	UNP P30411
R	461	VAL	-	expression tag	UNP P30411
R	462	ILE	-	expression tag	UNP P30411
R	463	LEU	-	expression tag	UNP P30411
R	464	PRO	-	expression tag	UNP P30411
R	465	TYR	-	expression tag	UNP P30411
R	466	GLY	-	expression tag	UNP P30411
R	467	THR	-	expression tag	UNP P30411
R	468	LEU	-	expression tag	UNP P30411
R	469	VAL	-	expression tag	UNP P30411
R	470	ILE	-	expression tag	UNP P30411
R	471	ASP	-	expression tag	UNP P30411
R	472	GLY	-	expression tag	UNP P30411
R	473	VAL	-	expression tag	UNP P30411
R	474	THR	-	expression tag	UNP P30411
R	475	PRO	-	expression tag	UNP P30411
R	476	ASN	-	expression tag	UNP P30411
R	477	MET	-	expression tag	UNP P30411
R	478	LEU	-	expression tag	UNP P30411
R	479	ASN	-	expression tag	UNP P30411
R	480	TYR	-	expression tag	UNP P30411
R	481	PHE	-	expression tag	UNP P30411

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Chain	Residue	Modelled	Actual	Comment	Reference
R	482	GLY	-	expression tag	UNP P30411
R	483	ARG	-	expression tag	UNP P30411
R	484	PRO	-	expression tag	UNP P30411
R	485	TYR	-	expression tag	UNP P30411
R	486	GLU	-	expression tag	UNP P30411
R	487	GLY	-	expression tag	UNP P30411
R	488	ILE	-	expression tag	UNP P30411
R	489	ALA	-	expression tag	UNP P30411
R	490	VAL	-	expression tag	UNP P30411
R	491	PHE	-	expression tag	UNP P30411
R	492	ASP	-	expression tag	UNP P30411
R	493	GLY	-	expression tag	UNP P30411
R	494	LYS	-	expression tag	UNP P30411
R	495	LYS	-	expression tag	UNP P30411
R	496	ILE	-	expression tag	UNP P30411
R	497	THR	-	expression tag	UNP P30411
R	498	VAL	-	expression tag	UNP P30411
R	499	THR	-	expression tag	UNP P30411
R	500	GLY	-	expression tag	UNP P30411
R	501	THR	-	expression tag	UNP P30411
R	502	LEU	-	expression tag	UNP P30411
R	503	TRP	-	expression tag	UNP P30411
R	504	ASN	-	expression tag	UNP P30411
R	505	GLY	-	expression tag	UNP P30411
R	506	ASN	-	expression tag	UNP P30411
R	507	LYS	-	expression tag	UNP P30411
R	508	ILE	-	expression tag	UNP P30411
R	509	ILE	-	expression tag	UNP P30411
R	510	ASP	-	expression tag	UNP P30411
R	511	GLU	-	expression tag	UNP P30411
R	512	ARG	-	expression tag	UNP P30411
R	513	LEU	-	expression tag	UNP P30411
R	514	ILE	-	expression tag	UNP P30411
R	515	THR	-	expression tag	UNP P30411
R	516	PRO	-	expression tag	UNP P30411
R	517	ASP	-	expression tag	UNP P30411
R	518	GLY	-	expression tag	UNP P30411
R	519	SER	-	expression tag	UNP P30411
R	520	MET	-	expression tag	UNP P30411
R	521	LEU	-	expression tag	UNP P30411
R	522	PHE	-	expression tag	UNP P30411
R	523	ARG	-	expression tag	UNP P30411

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Chain	Residue	Modelled	Actual	Comment	Reference
R	524	VAL	-	expression tag	UNP P30411
R	525	THR	-	expression tag	UNP P30411
R	526	ILE	-	expression tag	UNP P30411
R	527	ASN	-	expression tag	UNP P30411
R	528	SER	-	expression tag	UNP P30411

- Molecule 5 is a protein called single Fab chain (svFv16).

Mol	Chain	Residues	Atoms					AltConf	Trace
5	S	232	Total	C	N	O	S	0	0
			1784	1132	295	347	10		

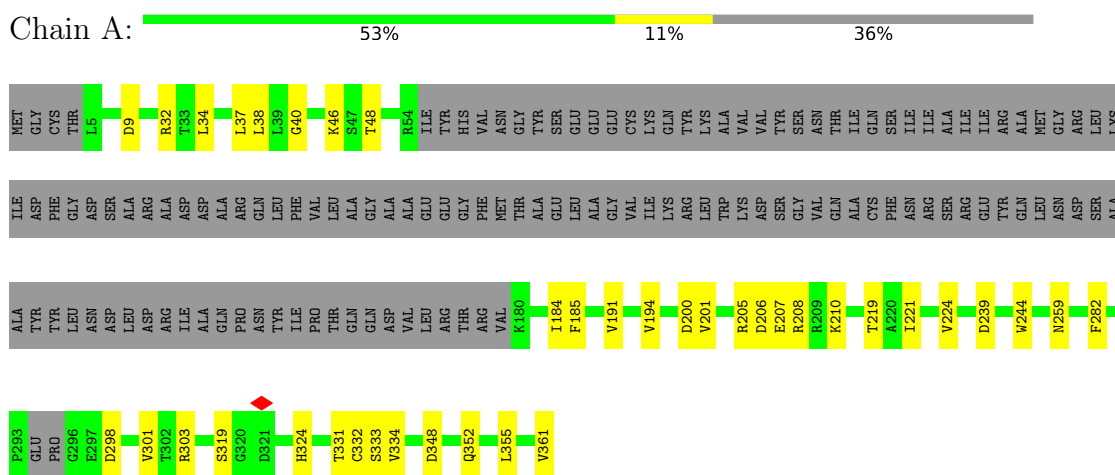
- Molecule 6 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	Y	51	Total	C	N	O	S	0	0
			353	222	60	69	2		

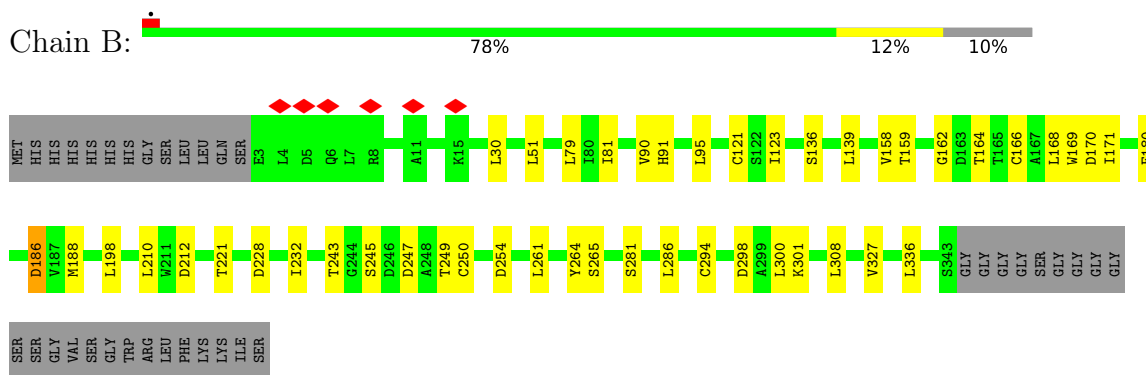
### 3 Residue-property plots [i](#)

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: G subunit q (Gil-Gq chimeric)



- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

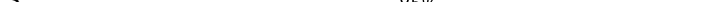


- Molecule 3: ARG-PRO-PRO-GLY-PHE-SER-PRO-PHE-ARG



- Molecule 4: B2 bradykinin receptor

THR	THR	ARG	GLY	C211	GLY	W55	PHE	ALA
PRO	ASP	VAL	GLY	L218	GLY	W65	ARG	LEU
ASN	MET	ARG	ARG	L219	CYS	W65	HIS	GLU
THR	ASN	SER	SER	W220	ASP	A71	PHE	ASP
PHE	THR	GLY	GLU	F233	GLU	N75	ILE	TRP
GLY	ASN	ASN	ILE	L237	ILE	T90	LEU	GLU
ARG	LEU	ALA	GLN	M248	MET	T90	THR	LEU
PRO	LEU	THR	GLY	W248	ARG	I94	GLY	ASN
THR	ILE	LYS	ASN	M248	ASN	I94	ILE	ASP
GLU	ASP	ASP	SER	Q257	SER	A101	ASP	ASP
ILE	ILE	THR	GLY	PHE	MET	A101	ASP	ASN
ALA	VAL	VAL	THR	LYS	THR	L104	ALA	LYS
VAL	VAL	ILE	LEU	GLY	LEU	I105	LEU	VAL
PHE	PHE	ILE	VAL	ILE	VAL	L106	LYS	ILE
ASP	ASP	PRO	PHE	Q263	PHE	A107	LEU	GLU
GLY	GLY	TYR	THR	THR	THR	L110	ALA	LYS
LYS	LYS	GLY	GLU	T269	LEU	L110	ASN	ASP
ILE	ILE	GLY	LEU	T270	GLY	W113	ASN	ASN
THR	THR	SER	PHE	L271	ASP	W119	LYS	ALA
ALA	ALA	ALA	VAL	V275	PHE	D122	VAL	ALA
ASP	ASP	ASP	GLY	P285	VAL	D122	GLY	GLN
GLY	GLY	GLN	ASP	F286	ASP	F125	GLU	VAL
THR	THR	MET	TRP	Q287	TRP	L129	GLM	LYS
LEU	LEU	ALA	GLU	I288	GLU	A134	ALA	ALA
TRP	TRP	GLN	GLN	T290	GLU	I136	LEU	ALA
ASN	ASN	ILE	ALA	T290	ALA	N140	THR	ALA
LYS	LYS	VAL	VAL	D293	TYR	L141	ARG	LEU
PHE	PHE	PHE	ASN	T294	ASN	A135	ASN	ASP
ILE	ILE	LYS	ASN	L295	LEU	I136	LYS	ALA
ASP	ASP	VAL	ASP	H296	ASP	N140	THR	ALA
GLU	GLU	VAL	GLN	R297	GLN	L141	THR	ALA
ARG	ARG	TYR	VAL	T297	VAL	L150	ARG	LEU
LEU	LEU	PRO	LEU	I313	VAL	I150	ASN	ASP
ILE	ILE	VAL	GLU	S318	VAL	I153	ALA	ALA
THR	THR	ASP	GLN	S318	GLN	D154	TYR	GLN
PRO	PRO	ASP	GLY	Y322	GLY	L157	ILE	LYS
ASP	ASP	HIS	GLY	Y322	GLY	A157	LYS	ALA
GLY	GLY	HIS	VAL	C326	VAL	A157	THR	PRO
SER	SER	PHE	SER	C326	SER	T162	LEU	LYS
MET	MET	LYS	SER	L330	LEU	M163	GLY	LYS
LEU	LEU	VAL	LEU	L330	LEU	M163	THR	LEU
PHE	PHE	ILE	LEU	I334	LEU	M163	PHE	GLU
ARG	ARG	LEU	GLN	I334	GLN	M163	ALA	GLU
VAL	VAL	PRO	ASN	V335	ASN	M165	ALA	LYS
THR	THR	TYR	LEU	V335	LEU	M165	GLM	SER
ILE	ILE	GLY	ALA	V346	LEU	R169	SER	LYS
ASN	ASN	THR	VAL	T346	VAL	R169	LYS	PRO
SER	SER	LEU	SER	THR	SER	R172	CYS	ASP
		VAL	VAL	GLN	GLY	R172	PRO	PRO
		VAL	VAL	GLY	VAL	G183	GLM	SER
		ILE	THR	VAL	THR	G183	VAL	GLU
		ASP	THR	CYS	CYS	L187	GLU	MET
		GLY	ILE	LYS	LYS	L187	TRP	LYS
		VAL	GLN	THR	THR	L187	LEU	ASP

- Chain S:  85% 8% 6%

The diagram illustrates the protein structure of the C-terminal domain of the human Hsp70 chaperone. The sequence is shown as a horizontal bar with residues labeled below it. The residues are color-coded: yellow for surface-exposed, green for buried, and grey for alpha-helical. Specific residues are highlighted with red diamonds: A136 and A143. The diagram also indicates the positions of H232, L247, and N169.

Residue	Type
D1	Buried
F29	Surface-exposed
G33	Buried
A40	Surface-exposed
K43	Surface-exposed
S52	Surface-exposed
A61	Buried
K65	Surface-exposed
R72	Surface-exposed
M83	Buried
L86	Surface-exposed
S99	Surface-exposed
I100	Surface-exposed
Y101	Buried
Y102	Buried
S105	Surface-exposed
S120	Buried
ALA	Alpha-helical
GLY	Alpha-helical
GLY	Alpha-helical
GLY	Alpha-helical
GLY	Alpha-helical
SER	Alpha-helical
GLY	Alpha-helical
GLY	Alpha-helical
GLY	Alpha-helical
SER	Alpha-helical
SER	Alpha-helical
GLY	Alpha-helical
GLY	Alpha-helical
GLY	Alpha-helical
SER	Alpha-helical
A136	Buried
A143	Buried
N169	Surface-exposed
L187	Surface-exposed
Y190	Surface-exposed
R202	Surface-exposed
D223	Surface-exposed

- Chain Y:  69% 28%

MET  
ALA  
SER  
ASN  
ASN  
THR  
ALA  
SER  
ILE  
ALA  
Q11  
K14  
E22  
A23  
D48  
F61  
ARG  
GLU  
LYS  
LYS  
PHE  
PHE  
CYS  
ALA  
ILE  
LEU

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	664416	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 ( $e^-/\text{\AA}^2$ )	80	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	OTHER	Depositor
Maximum map value	1.619	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.029	Depositor
Recommended contour level	0.01	Depositor
Map size ( $\text{\AA}$ )	208.99998, 208.99998, 208.99998	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.045, 1.045, 1.045	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	0.26	0/1910	0.43	0/2570
2	B	0.24	0/2652	0.47	0/3596
3	D	0.39	0/80	0.58	0/106
4	R	0.25	0/2362	0.43	0/3217
5	S	0.24	0/1828	0.44	0/2479
6	Y	0.24	0/359	0.39	0/492
All	All	0.25	0/9191	0.45	0/12460

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
4	R	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	R	322	TYR	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	1878	0	1856	24	0
2	B	2605	0	2506	34	0
3	D	76	0	75	7	0
4	R	2308	0	2386	33	0
5	S	1784	0	1723	11	0
6	Y	353	0	317	2	0
All	All	9004	0	8863	96	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 96 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:THR:HG21	1:A:333:SER:OG	1.75	0.86
1:A:210:LYS:NZ	2:B:228:ASP:OD2	2.19	0.73
1:A:205:ARG:NH2	1:A:207:GLU:OE2	2.29	0.66
2:B:90:VAL:HG13	5:S:102:TYR:HB2	1.81	0.62
4:R:293:ASP:OD1	4:R:297:ARG:NH2	2.32	0.62

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	224/361 (62%)	216 (96%)	8 (4%)	0	100	100
2	B	339/377 (90%)	325 (96%)	14 (4%)	0	100	100
3	D	7/9 (78%)	7 (100%)	0	0	100	100
4	R	283/595 (48%)	276 (98%)	7 (2%)	0	100	100
5	S	228/248 (92%)	221 (97%)	7 (3%)	0	100	100

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	Y	49/71 (69%)	49 (100%)	0	0	100	100
All	All	1130/1661 (68%)	1094 (97%)	36 (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	204/316 (65%)	201 (98%)	3 (2%)	60	85
2	B	280/308 (91%)	279 (100%)	1 (0%)	89	97
3	D	8/8 (100%)	8 (100%)	0	100	100
4	R	263/524 (50%)	259 (98%)	4 (2%)	60	85
5	S	196/199 (98%)	195 (100%)	1 (0%)	86	96
6	Y	31/58 (53%)	31 (100%)	0	100	100
All	All	982/1413 (70%)	973 (99%)	9 (1%)	74	92

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	R	295	LEU
5	S	232	HIS
2	B	186	ASP
4	R	65	TRP
4	R	218	LEU

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 [i](#)

There are no chain breaks in this entry.

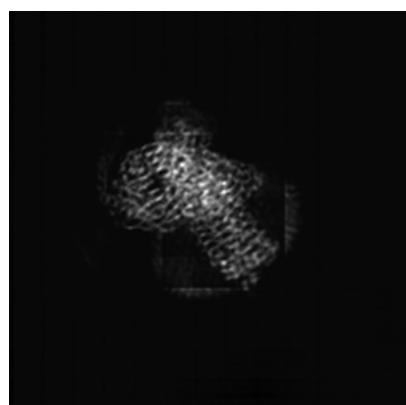
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31429. These allow visual inspection of the internal detail of the map and identification of artifacts.

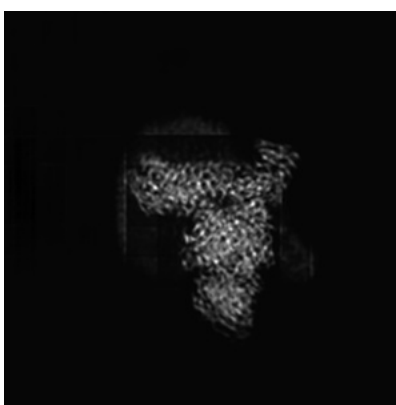
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

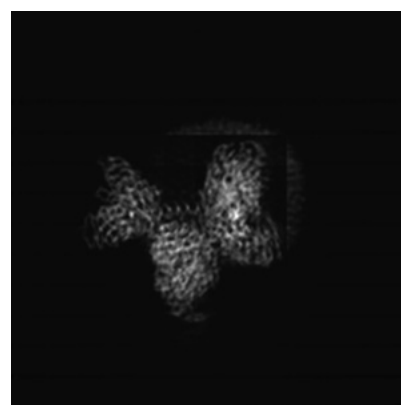
#### 6.1.1 Primary map



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: 100



Y Index: 100



Z Index: 100

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: 111



Y Index: 88

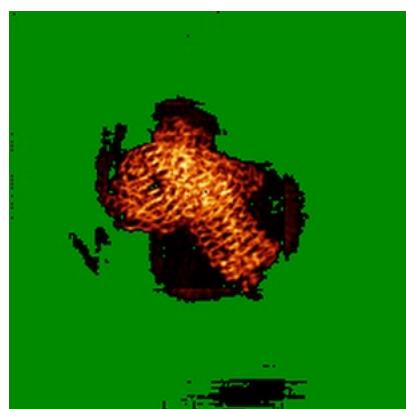


Z Index: 109

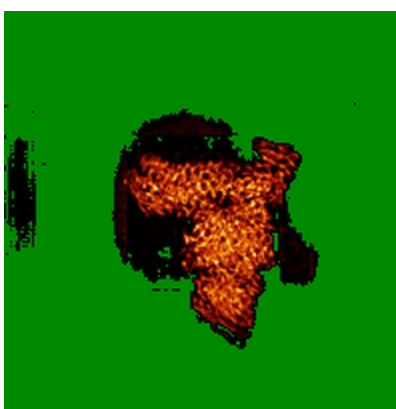
The images above show the largest variance slices of the map in three orthogonal directions.

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

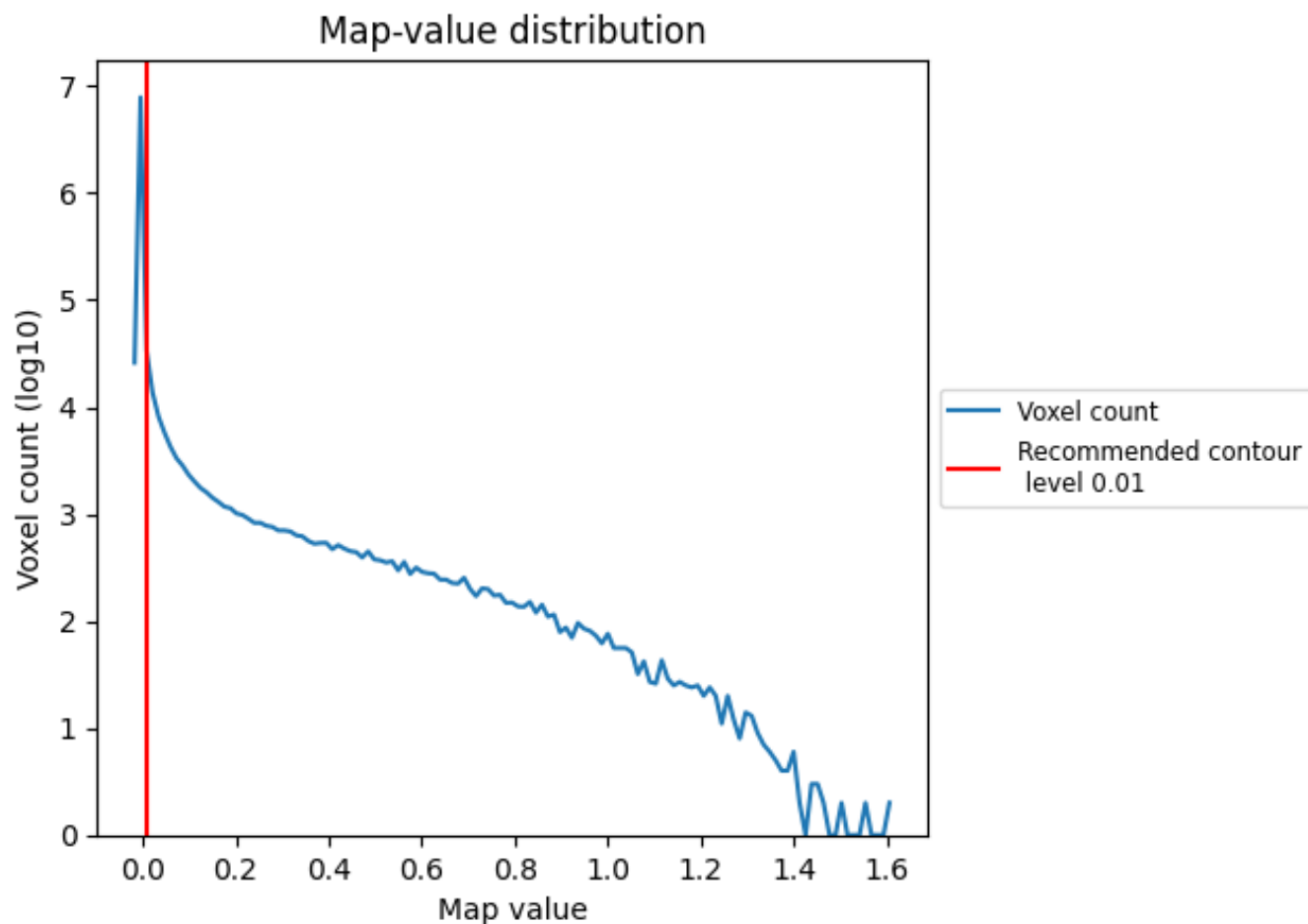
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

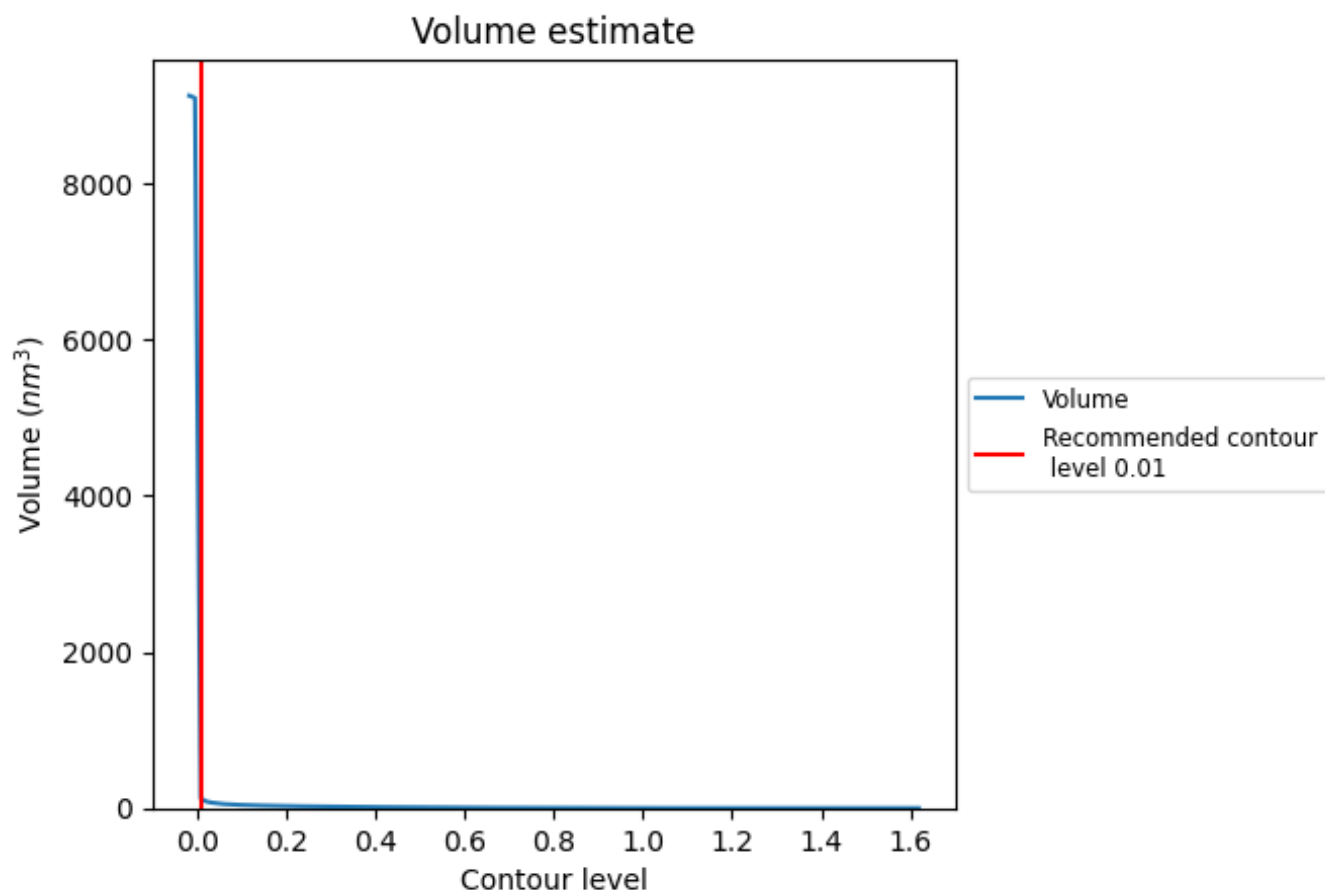
This section contains the results of statistical analysis of the map.

### 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.

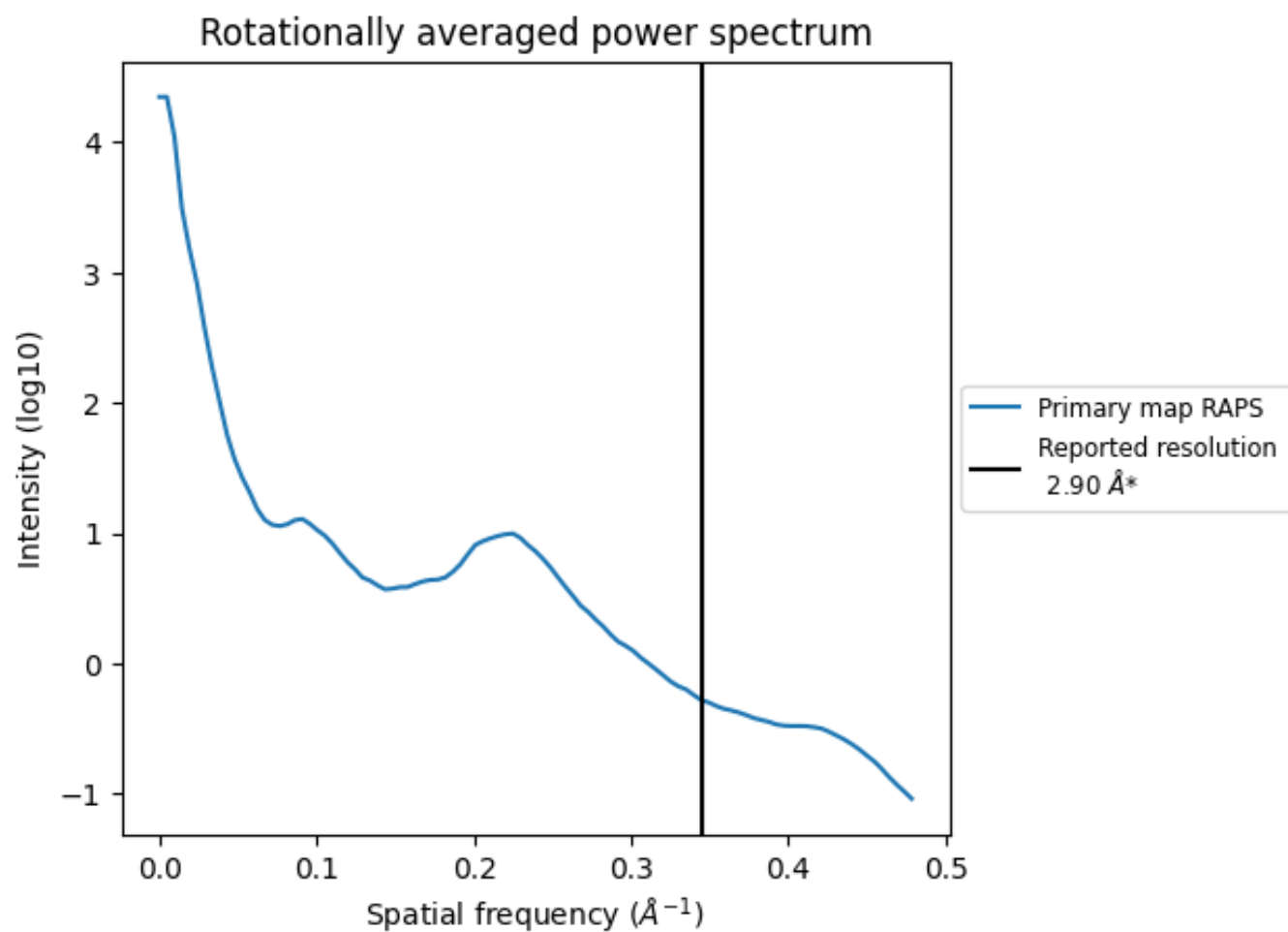
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm<sup>3</sup>; this corresponds to an approximate mass of 107 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 0.345 Å<sup>-1</sup>

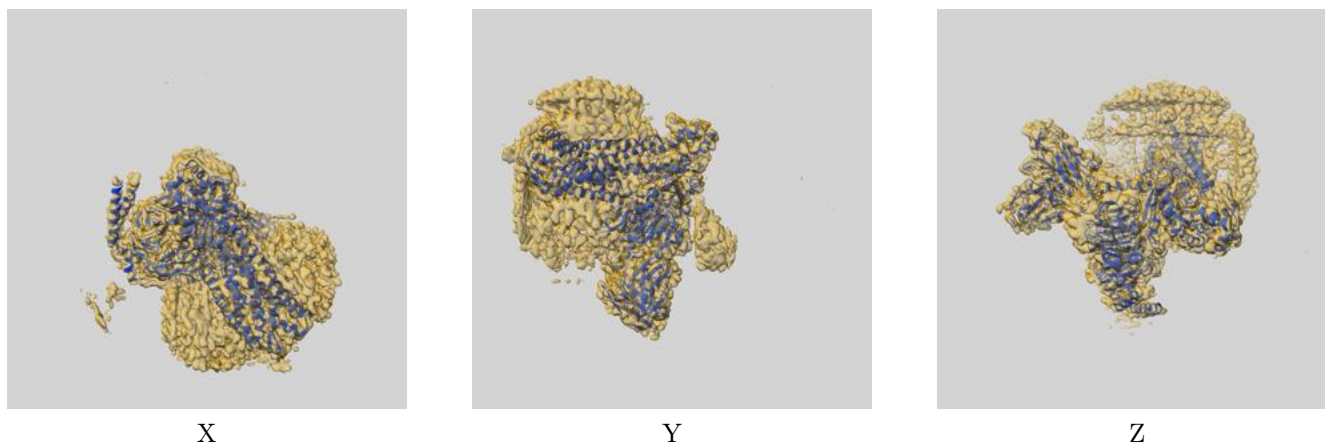
## 8 Fourier-Shell correlation ⓘ

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

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

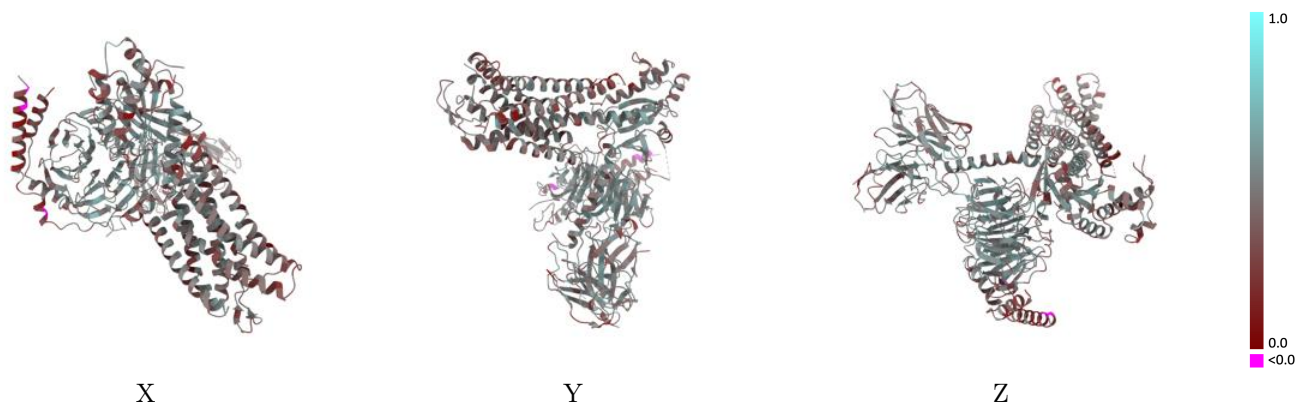
This section contains information regarding the fit between EMDB map EMD-31429 and PDB model 7F2O. Per-residue inclusion information can be found in section [3](#) on page [12](#).

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



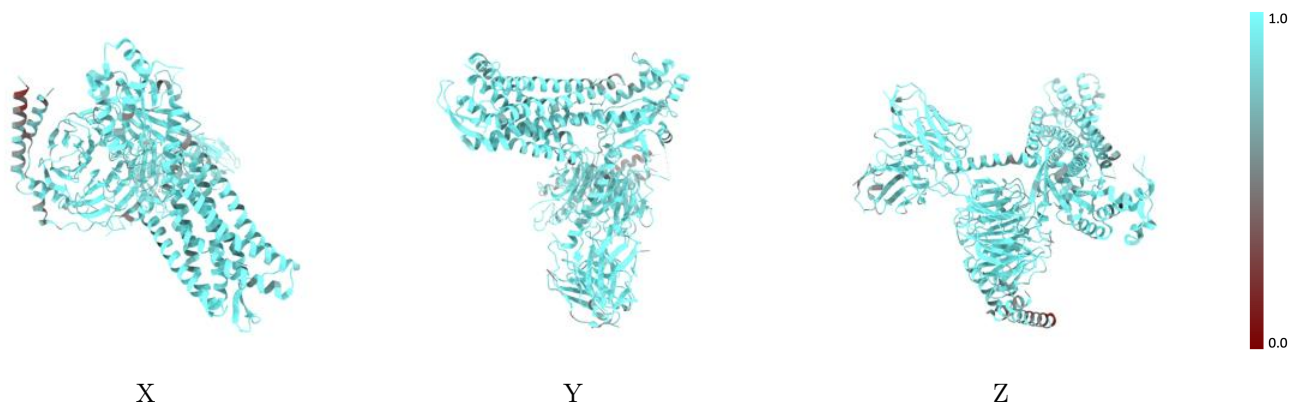
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



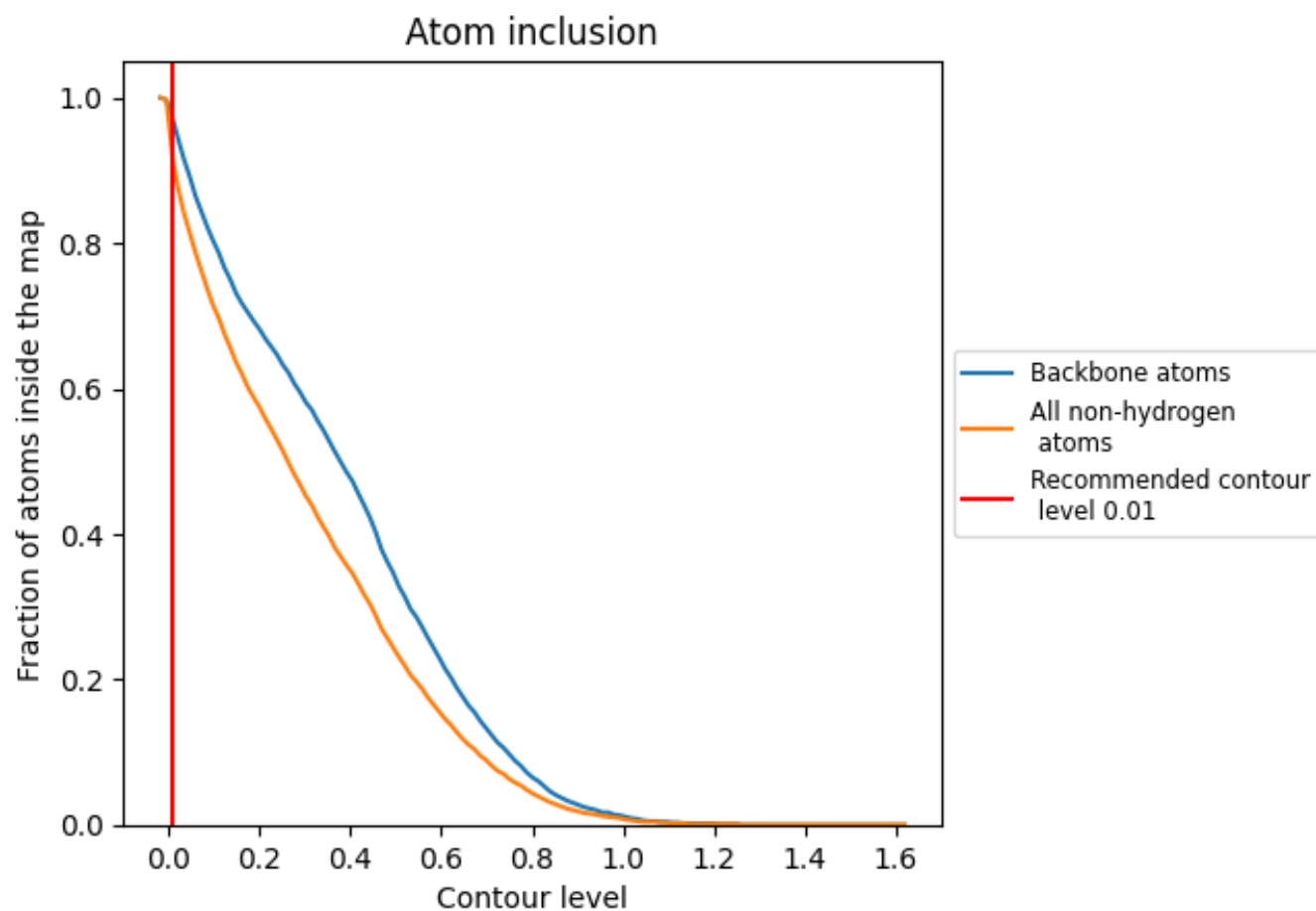
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 91% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div><div></div></div> 0.9120	<div><div></div></div> 0.4360
A	<div><div></div></div> 0.9130	<div><div></div></div> 0.4510
B	<div><div></div></div> 0.9140	<div><div></div></div> 0.4580
D	<div><div></div></div> 0.9580	<div><div></div></div> 0.3770
R	<div><div></div></div> 0.9130	<div><div></div></div> 0.3960
S	<div><div></div></div> 0.9120	<div><div></div></div> 0.4520
Y	<div><div></div></div> 0.8630	<div><div></div></div> 0.3870

1.0

0.0

<0.0