



## Full wwPDB EM Validation Report ⓘ

Nov 11, 2024 – 04:26 PM JST

PDB ID : 7EIB  
EMDB ID : EMD-31145  
Title : Cryo-EM structure of the type 1 bradykinin receptor in complex with the des-Arg10-kallidin and an Gq protein  
Authors : Yin, Y.; Jiang, Y.  
Deposited on : 2021-03-30  
Resolution : 3.00 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>.

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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

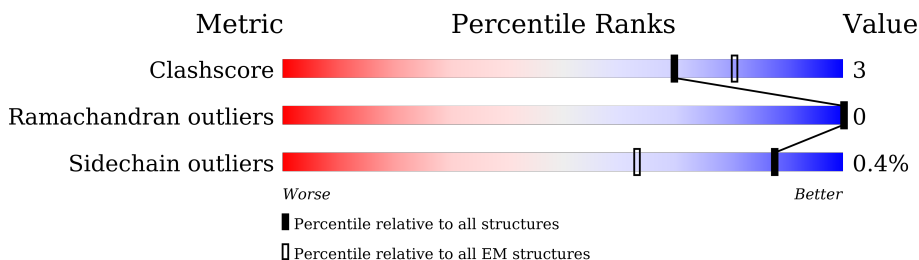
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.00 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	613	
2	D	9	
3	B	361	
4	C	377	
5	E	71	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7204 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 B1 bradykinin receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	295	Total	C	N	O	S	0	0
			2419	1621	409	381	8		

There are 265 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-104	ALA	-	expression tag	UNP P46663
A	-103	ASP	-	expression tag	UNP P46663
A	-102	LEU	-	expression tag	UNP P46663
A	-101	GLU	-	expression tag	UNP P46663
A	-100	ASP	-	expression tag	UNP P46663
A	-99	ASN	-	expression tag	UNP P46663
A	-98	TRP	-	expression tag	UNP P46663
A	-97	GLU	-	expression tag	UNP P46663
A	-96	THR	-	expression tag	UNP P46663
A	-95	LEU	-	expression tag	UNP P46663
A	-94	ASN	-	expression tag	UNP P46663
A	-93	ASP	-	expression tag	UNP P46663
A	-92	ASN	-	expression tag	UNP P46663
A	-91	LEU	-	expression tag	UNP P46663
A	-90	LYS	-	expression tag	UNP P46663
A	-89	VAL	-	expression tag	UNP P46663
A	-88	ILE	-	expression tag	UNP P46663
A	-87	GLU	-	expression tag	UNP P46663
A	-86	LYS	-	expression tag	UNP P46663
A	-85	ALA	-	expression tag	UNP P46663
A	-84	ASP	-	expression tag	UNP P46663
A	-83	ASN	-	expression tag	UNP P46663
A	-82	ALA	-	expression tag	UNP P46663
A	-81	ALA	-	expression tag	UNP P46663
A	-80	GLN	-	expression tag	UNP P46663
A	-79	VAL	-	expression tag	UNP P46663
A	-78	LYS	-	expression tag	UNP P46663
A	-77	ASP	-	expression tag	UNP P46663

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-76	ALA	-	expression tag	UNP P46663
A	-75	LEU	-	expression tag	UNP P46663
A	-74	THR	-	expression tag	UNP P46663
A	-73	LYS	-	expression tag	UNP P46663
A	-72	MET	-	expression tag	UNP P46663
A	-71	ARG	-	expression tag	UNP P46663
A	-70	ALA	-	expression tag	UNP P46663
A	-69	ALA	-	expression tag	UNP P46663
A	-68	ALA	-	expression tag	UNP P46663
A	-67	LEU	-	expression tag	UNP P46663
A	-66	ASP	-	expression tag	UNP P46663
A	-65	ALA	-	expression tag	UNP P46663
A	-64	GLN	-	expression tag	UNP P46663
A	-63	LYS	-	expression tag	UNP P46663
A	-62	ALA	-	expression tag	UNP P46663
A	-61	THR	-	expression tag	UNP P46663
A	-60	PRO	-	expression tag	UNP P46663
A	-59	PRO	-	expression tag	UNP P46663
A	-58	LYS	-	expression tag	UNP P46663
A	-57	LEU	-	expression tag	UNP P46663
A	-56	GLU	-	expression tag	UNP P46663
A	-55	ASP	-	expression tag	UNP P46663
A	-54	LYS	-	expression tag	UNP P46663
A	-53	SER	-	expression tag	UNP P46663
A	-52	PRO	-	expression tag	UNP P46663
A	-51	ASP	-	expression tag	UNP P46663
A	-50	SER	-	expression tag	UNP P46663
A	-49	PRO	-	expression tag	UNP P46663
A	-48	GLU	-	expression tag	UNP P46663
A	-47	MET	-	expression tag	UNP P46663
A	-46	LYS	-	expression tag	UNP P46663
A	-45	ASP	-	expression tag	UNP P46663
A	-44	PHE	-	expression tag	UNP P46663
A	-43	ARG	-	expression tag	UNP P46663
A	-42	HIS	-	expression tag	UNP P46663
A	-41	GLY	-	expression tag	UNP P46663
A	-40	PHE	-	expression tag	UNP P46663
A	-39	ASP	-	expression tag	UNP P46663
A	-38	ILE	-	expression tag	UNP P46663
A	-37	LEU	-	expression tag	UNP P46663
A	-36	VAL	-	expression tag	UNP P46663
A	-35	GLY	-	expression tag	UNP P46663

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-34	GLN	-	expression tag	UNP P46663
A	-33	ILE	-	expression tag	UNP P46663
A	-32	ASP	-	expression tag	UNP P46663
A	-31	ASP	-	expression tag	UNP P46663
A	-30	ALA	-	expression tag	UNP P46663
A	-29	LEU	-	expression tag	UNP P46663
A	-28	LYS	-	expression tag	UNP P46663
A	-27	LEU	-	expression tag	UNP P46663
A	-26	ALA	-	expression tag	UNP P46663
A	-25	ASN	-	expression tag	UNP P46663
A	-24	GLU	-	expression tag	UNP P46663
A	-23	GLY	-	expression tag	UNP P46663
A	-22	LYS	-	expression tag	UNP P46663
A	-21	VAL	-	expression tag	UNP P46663
A	-20	LYS	-	expression tag	UNP P46663
A	-19	GLU	-	expression tag	UNP P46663
A	-18	ALA	-	expression tag	UNP P46663
A	-17	GLN	-	expression tag	UNP P46663
A	-16	ALA	-	expression tag	UNP P46663
A	-15	ALA	-	expression tag	UNP P46663
A	-14	ALA	-	expression tag	UNP P46663
A	-13	GLU	-	expression tag	UNP P46663
A	-12	GLN	-	expression tag	UNP P46663
A	-11	LEU	-	expression tag	UNP P46663
A	-10	LYS	-	expression tag	UNP P46663
A	-9	THR	-	expression tag	UNP P46663
A	-8	THR	-	expression tag	UNP P46663
A	-7	ARG	-	expression tag	UNP P46663
A	-6	ASN	-	expression tag	UNP P46663
A	-5	ALA	-	expression tag	UNP P46663
A	-4	TYR	-	expression tag	UNP P46663
A	-3	ILE	-	expression tag	UNP P46663
A	-2	GLN	-	expression tag	UNP P46663
A	-1	LYS	-	expression tag	UNP P46663
A	0	TYR	-	expression tag	UNP P46663
A	1	LEU	-	expression tag	UNP P46663
A	126	TRP	PHE	engineered mutation	UNP P46663
A	351	VAL	-	expression tag	UNP P46663
A	352	PHE	-	expression tag	UNP P46663
A	353	THR	-	expression tag	UNP P46663
A	354	LEU	-	expression tag	UNP P46663
A	355	GLU	-	expression tag	UNP P46663

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Chain	Residue	Modelled	Actual	Comment	Reference
A	356	ASP	-	expression tag	UNP P46663
A	357	PHE	-	expression tag	UNP P46663
A	358	VAL	-	expression tag	UNP P46663
A	359	GLY	-	expression tag	UNP P46663
A	360	ASP	-	expression tag	UNP P46663
A	361	TRP	-	expression tag	UNP P46663
A	362	GLU	-	expression tag	UNP P46663
A	363	GLN	-	expression tag	UNP P46663
A	364	THR	-	expression tag	UNP P46663
A	365	ALA	-	expression tag	UNP P46663
A	366	ALA	-	expression tag	UNP P46663
A	367	TYR	-	expression tag	UNP P46663
A	368	ASN	-	expression tag	UNP P46663
A	369	LEU	-	expression tag	UNP P46663
A	370	ASP	-	expression tag	UNP P46663
A	371	GLN	-	expression tag	UNP P46663
A	372	VAL	-	expression tag	UNP P46663
A	373	LEU	-	expression tag	UNP P46663
A	374	GLU	-	expression tag	UNP P46663
A	375	GLN	-	expression tag	UNP P46663
A	376	GLY	-	expression tag	UNP P46663
A	377	GLY	-	expression tag	UNP P46663
A	378	VAL	-	expression tag	UNP P46663
A	379	SER	-	expression tag	UNP P46663
A	380	SER	-	expression tag	UNP P46663
A	381	LEU	-	expression tag	UNP P46663
A	382	LEU	-	expression tag	UNP P46663
A	383	GLN	-	expression tag	UNP P46663
A	384	ASN	-	expression tag	UNP P46663
A	385	LEU	-	expression tag	UNP P46663
A	386	ALA	-	expression tag	UNP P46663
A	387	VAL	-	expression tag	UNP P46663
A	388	SER	-	expression tag	UNP P46663
A	389	VAL	-	expression tag	UNP P46663
A	390	THR	-	expression tag	UNP P46663
A	391	PRO	-	expression tag	UNP P46663
A	392	ILE	-	expression tag	UNP P46663
A	393	GLN	-	expression tag	UNP P46663
A	394	ARG	-	expression tag	UNP P46663
A	395	ILE	-	expression tag	UNP P46663
A	396	VAL	-	expression tag	UNP P46663
A	397	ARG	-	expression tag	UNP P46663

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Chain	Residue	Modelled	Actual	Comment	Reference
A	398	SER	-	expression tag	UNP P46663
A	399	GLY	-	expression tag	UNP P46663
A	400	GLU	-	expression tag	UNP P46663
A	401	ASN	-	expression tag	UNP P46663
A	402	ALA	-	expression tag	UNP P46663
A	403	LEU	-	expression tag	UNP P46663
A	404	LYS	-	expression tag	UNP P46663
A	405	ILE	-	expression tag	UNP P46663
A	406	ASP	-	expression tag	UNP P46663
A	407	ILE	-	expression tag	UNP P46663
A	408	HIS	-	expression tag	UNP P46663
A	409	VAL	-	expression tag	UNP P46663
A	410	ILE	-	expression tag	UNP P46663
A	411	ILE	-	expression tag	UNP P46663
A	412	PRO	-	expression tag	UNP P46663
A	413	TYR	-	expression tag	UNP P46663
A	414	GLU	-	expression tag	UNP P46663
A	415	GLY	-	expression tag	UNP P46663
A	416	LEU	-	expression tag	UNP P46663
A	417	SER	-	expression tag	UNP P46663
A	418	ALA	-	expression tag	UNP P46663
A	419	ASP	-	expression tag	UNP P46663
A	420	GLN	-	expression tag	UNP P46663
A	421	MET	-	expression tag	UNP P46663
A	422	ALA	-	expression tag	UNP P46663
A	423	GLN	-	expression tag	UNP P46663
A	424	ILE	-	expression tag	UNP P46663
A	425	GLU	-	expression tag	UNP P46663
A	426	GLU	-	expression tag	UNP P46663
A	427	VAL	-	expression tag	UNP P46663
A	428	PHE	-	expression tag	UNP P46663
A	429	LYS	-	expression tag	UNP P46663
A	430	VAL	-	expression tag	UNP P46663
A	431	VAL	-	expression tag	UNP P46663
A	432	TYR	-	expression tag	UNP P46663
A	433	PRO	-	expression tag	UNP P46663
A	434	VAL	-	expression tag	UNP P46663
A	435	ASP	-	expression tag	UNP P46663
A	436	ASP	-	expression tag	UNP P46663
A	437	HIS	-	expression tag	UNP P46663
A	438	HIS	-	expression tag	UNP P46663
A	439	PHE	-	expression tag	UNP P46663

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Chain	Residue	Modelled	Actual	Comment	Reference
A	440	LYS	-	expression tag	UNP P46663
A	441	VAL	-	expression tag	UNP P46663
A	442	ILE	-	expression tag	UNP P46663
A	443	LEU	-	expression tag	UNP P46663
A	444	PRO	-	expression tag	UNP P46663
A	445	TYR	-	expression tag	UNP P46663
A	446	GLY	-	expression tag	UNP P46663
A	447	THR	-	expression tag	UNP P46663
A	448	LEU	-	expression tag	UNP P46663
A	449	VAL	-	expression tag	UNP P46663
A	450	ILE	-	expression tag	UNP P46663
A	451	ASP	-	expression tag	UNP P46663
A	452	GLY	-	expression tag	UNP P46663
A	453	VAL	-	expression tag	UNP P46663
A	454	THR	-	expression tag	UNP P46663
A	455	PRO	-	expression tag	UNP P46663
A	456	ASN	-	expression tag	UNP P46663
A	457	MET	-	expression tag	UNP P46663
A	458	LEU	-	expression tag	UNP P46663
A	459	ASN	-	expression tag	UNP P46663
A	460	TYR	-	expression tag	UNP P46663
A	461	PHE	-	expression tag	UNP P46663
A	462	GLY	-	expression tag	UNP P46663
A	463	ARG	-	expression tag	UNP P46663
A	464	PRO	-	expression tag	UNP P46663
A	465	TYR	-	expression tag	UNP P46663
A	466	GLU	-	expression tag	UNP P46663
A	467	GLY	-	expression tag	UNP P46663
A	468	ILE	-	expression tag	UNP P46663
A	469	ALA	-	expression tag	UNP P46663
A	470	VAL	-	expression tag	UNP P46663
A	471	PHE	-	expression tag	UNP P46663
A	472	ASP	-	expression tag	UNP P46663
A	473	GLY	-	expression tag	UNP P46663
A	474	LYS	-	expression tag	UNP P46663
A	475	LYS	-	expression tag	UNP P46663
A	476	ILE	-	expression tag	UNP P46663
A	477	THR	-	expression tag	UNP P46663
A	478	VAL	-	expression tag	UNP P46663
A	479	THR	-	expression tag	UNP P46663
A	480	GLY	-	expression tag	UNP P46663
A	481	THR	-	expression tag	UNP P46663

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Chain	Residue	Modelled	Actual	Comment	Reference
A	482	LEU	-	expression tag	UNP P46663
A	483	TRP	-	expression tag	UNP P46663
A	484	ASN	-	expression tag	UNP P46663
A	485	GLY	-	expression tag	UNP P46663
A	486	ASN	-	expression tag	UNP P46663
A	487	LYS	-	expression tag	UNP P46663
A	488	ILE	-	expression tag	UNP P46663
A	489	ILE	-	expression tag	UNP P46663
A	490	ASP	-	expression tag	UNP P46663
A	491	GLU	-	expression tag	UNP P46663
A	492	ARG	-	expression tag	UNP P46663
A	493	LEU	-	expression tag	UNP P46663
A	494	ILE	-	expression tag	UNP P46663
A	495	THR	-	expression tag	UNP P46663
A	496	PRO	-	expression tag	UNP P46663
A	497	ASP	-	expression tag	UNP P46663
A	498	GLY	-	expression tag	UNP P46663
A	499	SER	-	expression tag	UNP P46663
A	500	MET	-	expression tag	UNP P46663
A	501	LEU	-	expression tag	UNP P46663
A	502	PHE	-	expression tag	UNP P46663
A	503	ARG	-	expression tag	UNP P46663
A	504	VAL	-	expression tag	UNP P46663
A	505	THR	-	expression tag	UNP P46663
A	506	ILE	-	expression tag	UNP P46663
A	507	ASN	-	expression tag	UNP P46663
A	508	SER	-	expression tag	UNP P46663

- Molecule 2 is a protein called LYS-ARG-PRO-PRO-GLY-PHE-SER-PRO-PHE.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	D	9	Total	C	N	O	0	0
			74	50	13	11		

- Molecule 3 is a protein called G subunit q (Gi1-Gq chimeric).

Mol	Chain	Residues	Atoms					AltConf	Trace
3	B	235	Total	C	N	O	S	0	0
			1880	1195	331	346	8		

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	338	Total	C	N	O	S	0	0
			2478	1540	440	479	19		

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	MET	-	initiating methionine	UNP P54311
C	-9	HIS	-	expression tag	UNP P54311
C	-8	HIS	-	expression tag	UNP P54311
C	-7	HIS	-	expression tag	UNP P54311
C	-6	HIS	-	expression tag	UNP P54311
C	-5	HIS	-	expression tag	UNP P54311
C	-4	HIS	-	expression tag	UNP P54311
C	-3	GLY	-	expression tag	UNP P54311
C	-2	SER	-	expression tag	UNP P54311
C	-1	LEU	-	expression tag	UNP P54311
C	0	LEU	-	expression tag	UNP P54311
C	1	GLN	-	expression tag	UNP P54311
C	341	GLY	-	expression tag	UNP P54311
C	342	SER	-	expression tag	UNP P54311
C	343	SER	-	expression tag	UNP P54311
C	344	GLY	-	expression tag	UNP P54311
C	345	GLY	-	expression tag	UNP P54311
C	346	GLY	-	expression tag	UNP P54311
C	347	GLY	-	expression tag	UNP P54311
C	348	SER	-	expression tag	UNP P54311
C	349	GLY	-	expression tag	UNP P54311
C	350	GLY	-	expression tag	UNP P54311
C	351	GLY	-	expression tag	UNP P54311
C	352	GLY	-	expression tag	UNP P54311
C	353	SER	-	expression tag	UNP P54311
C	354	SER	-	expression tag	UNP P54311
C	355	GLY	-	expression tag	UNP P54311
C	356	VAL	-	expression tag	UNP P54311
C	357	SER	-	expression tag	UNP P54311
C	358	GLY	-	expression tag	UNP P54311
C	359	TRP	-	expression tag	UNP P54311
C	360	ARG	-	expression tag	UNP P54311
C	361	LEU	-	expression tag	UNP P54311
C	362	PHE	-	expression tag	UNP P54311
C	363	LYS	-	expression tag	UNP P54311
C	364	LYS	-	expression tag	UNP P54311
C	365	ILE	-	expression tag	UNP P54311

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Chain	Residue	Modelled	Actual	Comment	Reference
C	366	SER	-	expression tag	UNP P54311

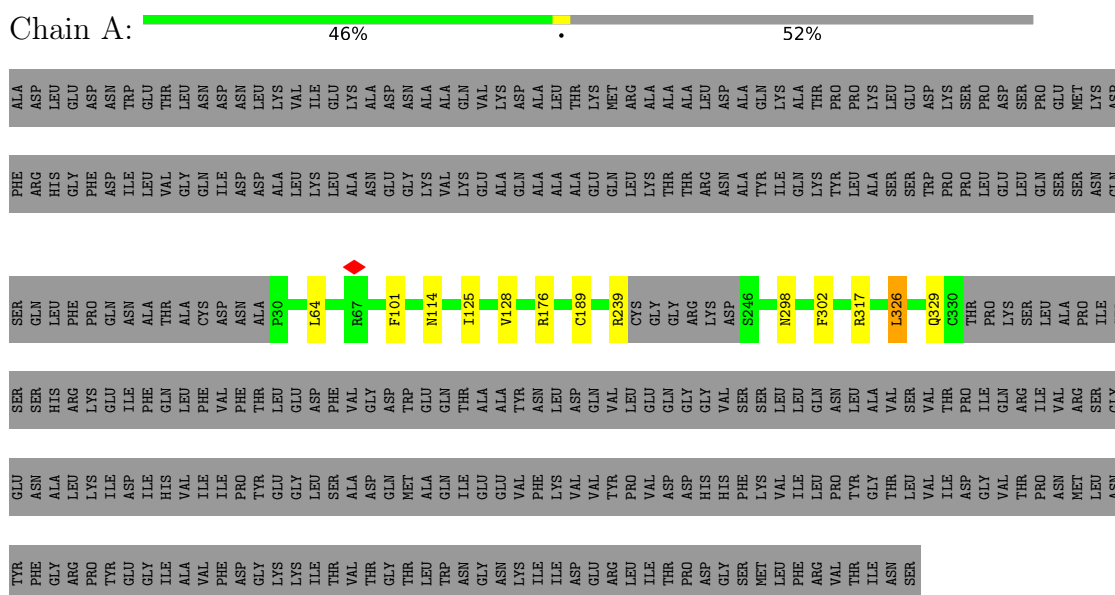
- Molecule 5 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

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

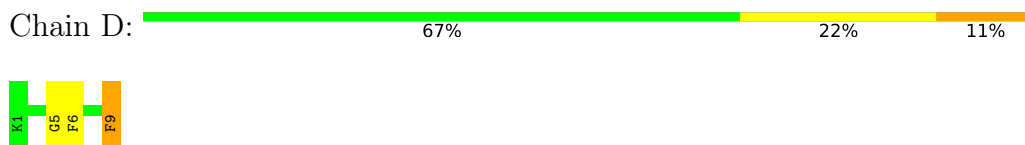
### 3 Residue-property plots

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.

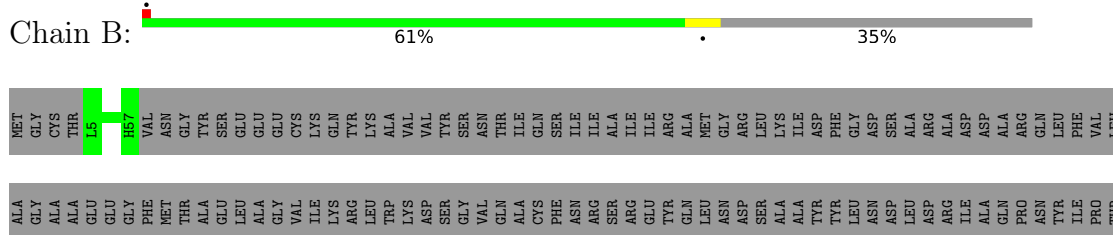
- Molecule 1: B1 bradykinin receptor



- Molecule 2: LYS-ARG-PRO-PRO-GLY-PHE-SER-PRO-PHE

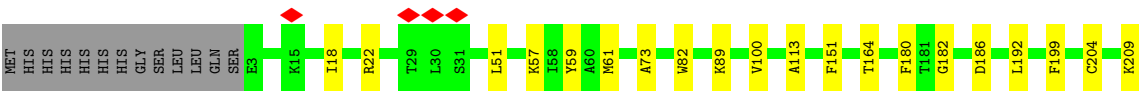
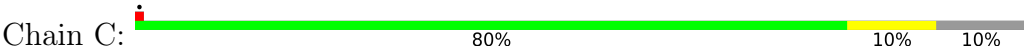


- Molecule 3: G subunit q (Gi1-Gq chimeric)

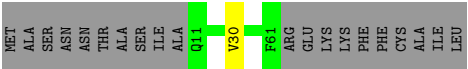




- Molecule 4: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1



- Molecule 5: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	633636	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 ( $e^-/\text{\AA}^2$ )	61.8	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	OTHER	Depositor
Maximum map value	1.714	Depositor
Minimum map value	-0.017	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.01	Depositor
Map size ( $\text{\AA}$ )	216.00002, 216.00002, 216.00002	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.08, 1.08, 1.08	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	0.29	0/2489	0.50	0/3396
2	D	1.52	0/78	1.03	0/103
3	B	0.32	0/1916	0.51	1/2587 (0.0%)
4	C	0.28	0/2524	0.57	0/3439
5	E	0.24	0/359	0.41	0/492
All	All	0.33	0/7366	0.53	1/10017 (0.0%)

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
1	A	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	295	PRO	CA-N-CD	-8.16	100.07	111.50

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	326	LEU	Mainchain

### 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	2419	0	2491	14	0
2	D	74	0	75	10	0
3	B	1880	0	1830	13	0
4	C	2478	0	2302	23	0
5	E	353	0	317	1	0
All	All	7204	0	7015	48	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 3.

All (48) 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)
3:B:293:PRO:HB2	3:B:295:PRO:HD2	1.42	0.99
1:A:101:PHE:CD1	2:D:6:PHE:CE2	2.79	0.71
1:A:298:ASN:HD21	2:D:9:PHE:H	1.39	0.70
3:B:216:ASN:HA	3:B:252:ILE:HD11	1.72	0.70
1:A:101:PHE:CD1	2:D:6:PHE:HE2	2.15	0.62
3:B:294:GLU:N	3:B:295:PRO:CD	2.63	0.61
1:A:176:ARG:NH1	2:D:5:GLY:O	2.33	0.60
4:C:251:ARG:NH1	4:C:260:GLU:OE1	2.32	0.57
1:A:101:PHE:CE1	2:D:6:PHE:HE2	2.24	0.56
1:A:114:ASN:ND2	1:A:189:CYS:SG	2.81	0.53
3:B:215:PHE:O	3:B:218:VAL:HG22	2.08	0.53
4:C:292:PHE:HA	4:C:314:ARG:HA	1.90	0.52
4:C:82:TRP:CH2	4:C:89:LYS:HE3	2.44	0.52
4:C:61:MET:HE1	4:C:328:ALA:HB3	1.92	0.51
1:A:326:LEU:HA	1:A:329:GLN:HG2	1.93	0.51
4:C:237:ASN:ND2	4:C:239:ASN:HD22	2.09	0.50
4:C:286:LEU:HD22	4:C:327:VAL:HG21	1.94	0.50
2:D:9:PHE:N	2:D:9:PHE:CD1	2.78	0.49
4:C:290:ASP:HA	4:C:314:ARG:HB2	1.94	0.49
3:B:205:ARG:NH1	4:C:186:ASP:OD1	2.43	0.48
3:B:208:ARG:NH2	3:B:239:ASP:OD1	2.31	0.48
4:C:164:THR:O	4:C:164:THR:HG22	2.13	0.48
4:C:308:LEU:HD23	4:C:339:TRP:CE2	2.49	0.48
1:A:302:PHE:CZ	2:D:9:PHE:HE1	2.32	0.47
1:A:317:ARG:NH2	3:B:361:VAL:O	2.44	0.47
4:C:271:CYS:HB3	4:C:290:ASP:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:293:PRO:CB	3:B:295:PRO:HD2	2.29	0.46
4:C:182:GLY:O	4:C:209:LYS:NZ	2.37	0.46
3:B:294:GLU:N	3:B:295:PRO:HD3	2.30	0.45
1:A:101:PHE:CG	2:D:6:PHE:CE2	3.03	0.45
4:C:180:PHE:CE1	4:C:216:GLY:HA2	2.51	0.44
4:C:192:LEU:HD23	4:C:199:PHE:HB3	1.98	0.44
1:A:101:PHE:CE1	2:D:6:PHE:CE2	3.03	0.44
4:C:51:LEU:HD23	4:C:82:TRP:CG	2.53	0.44
1:A:125:ILE:O	1:A:128:VAL:HG22	2.18	0.43
1:A:298:ASN:ND2	2:D:9:PHE:H	2.12	0.43
3:B:210:LYS:NZ	4:C:228:ASP:OD2	2.50	0.42
3:B:293:PRO:HB2	3:B:295:PRO:CD	2.30	0.42
4:C:186:ASP:HB2	4:C:204:CYS:SG	2.60	0.42
3:B:243:ILE:HG23	3:B:249:LEU:HD23	2.02	0.41
4:C:18:ILE:O	4:C:22:ARG:HG3	2.21	0.41
4:C:271:CYS:SG	4:C:290:ASP:HB2	2.61	0.41
1:A:64:LEU:HD23	1:A:326:LEU:HD12	2.01	0.41
4:C:57:LYS:HE2	4:C:59:TYR:OH	2.21	0.40
4:C:73:ALA:HB1	4:C:100:VAL:HG11	2.04	0.40
4:C:113:ALA:HB2	4:C:151:PHE:CZ	2.57	0.40
3:B:293:PRO:C	3:B:295:PRO:HD2	2.42	0.40
4:C:257:ALA:HB1	5:E:30:VAL:HG22	2.02	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	291/613 (48%)	288 (99%)	3 (1%)	0	100	100
2	D	7/9 (78%)	7 (100%)	0	0	100	100
3	B	231/361 (64%)	226 (98%)	5 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	C	336/377 (89%)	326 (97%)	10 (3%)	0	100	100
5	E	49/71 (69%)	49 (100%)	0	0	100	100
All	All	914/1431 (64%)	896 (98%)	18 (2%)	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	259/530 (49%)	258 (100%)	1 (0%)	89	95
2	D	8/8 (100%)	7 (88%)	1 (12%)	3	17
3	B	198/316 (63%)	197 (100%)	1 (0%)	86	94
4	C	248/308 (80%)	248 (100%)	0	100	100
5	E	31/58 (53%)	31 (100%)	0	100	100
All	All	744/1220 (61%)	741 (100%)	3 (0%)	88	95

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	239	ARG
2	D	9	PHE
3	B	358	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	ASN
4	C	237	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](#)

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.

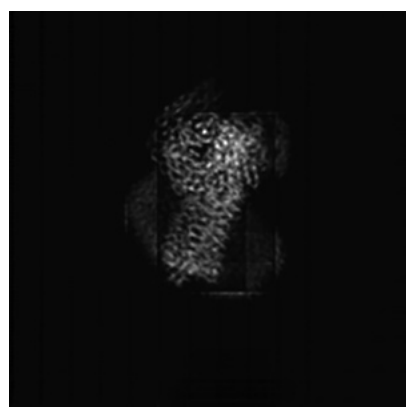
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31145. These allow visual inspection of the internal detail of the map and identification of artifacts.

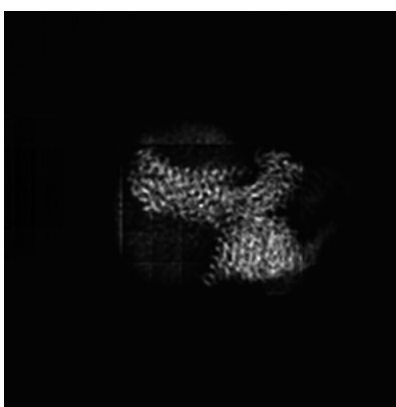
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

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

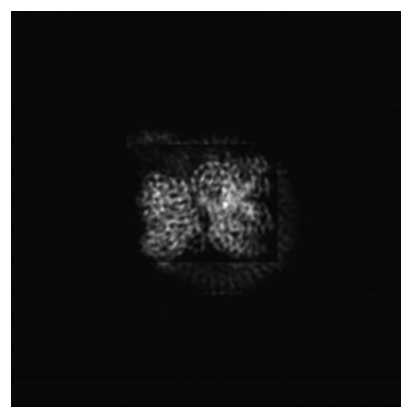
#### 6.1.1 Primary map



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

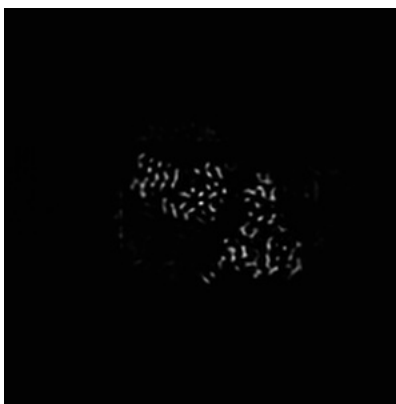
The images above show central slices of the map in three orthogonal directions.

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

### 6.3.1 Primary map



X Index: 109



Y Index: 103

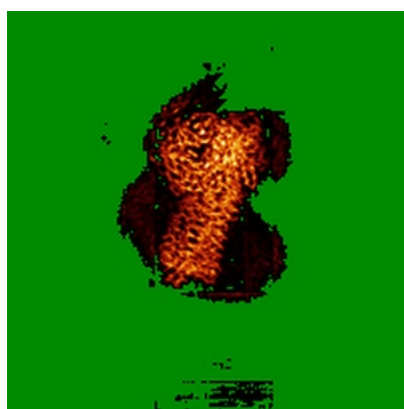


Z Index: 133

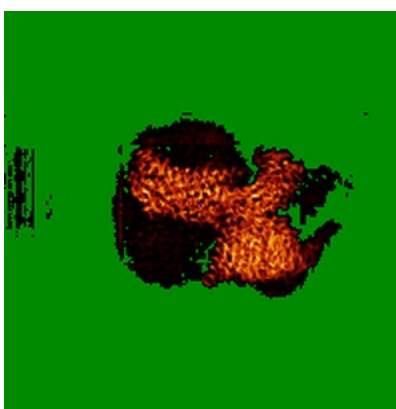
The images above show the largest variance slices of the map in three orthogonal directions.

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

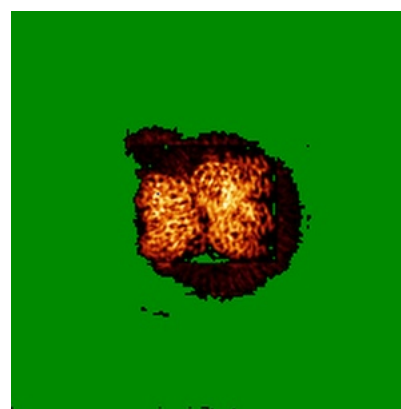
### 6.4.1 Primary map



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](#)

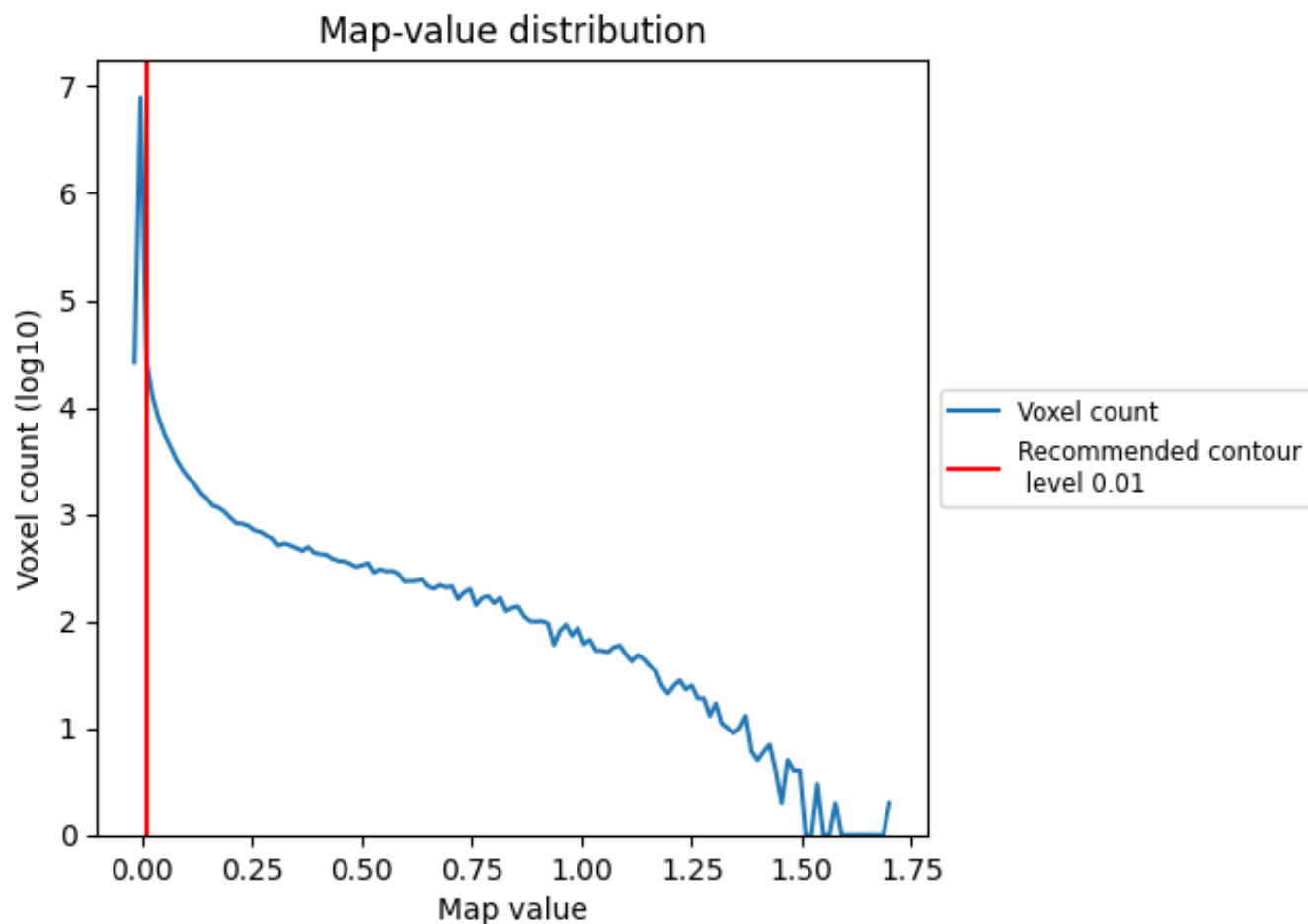
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

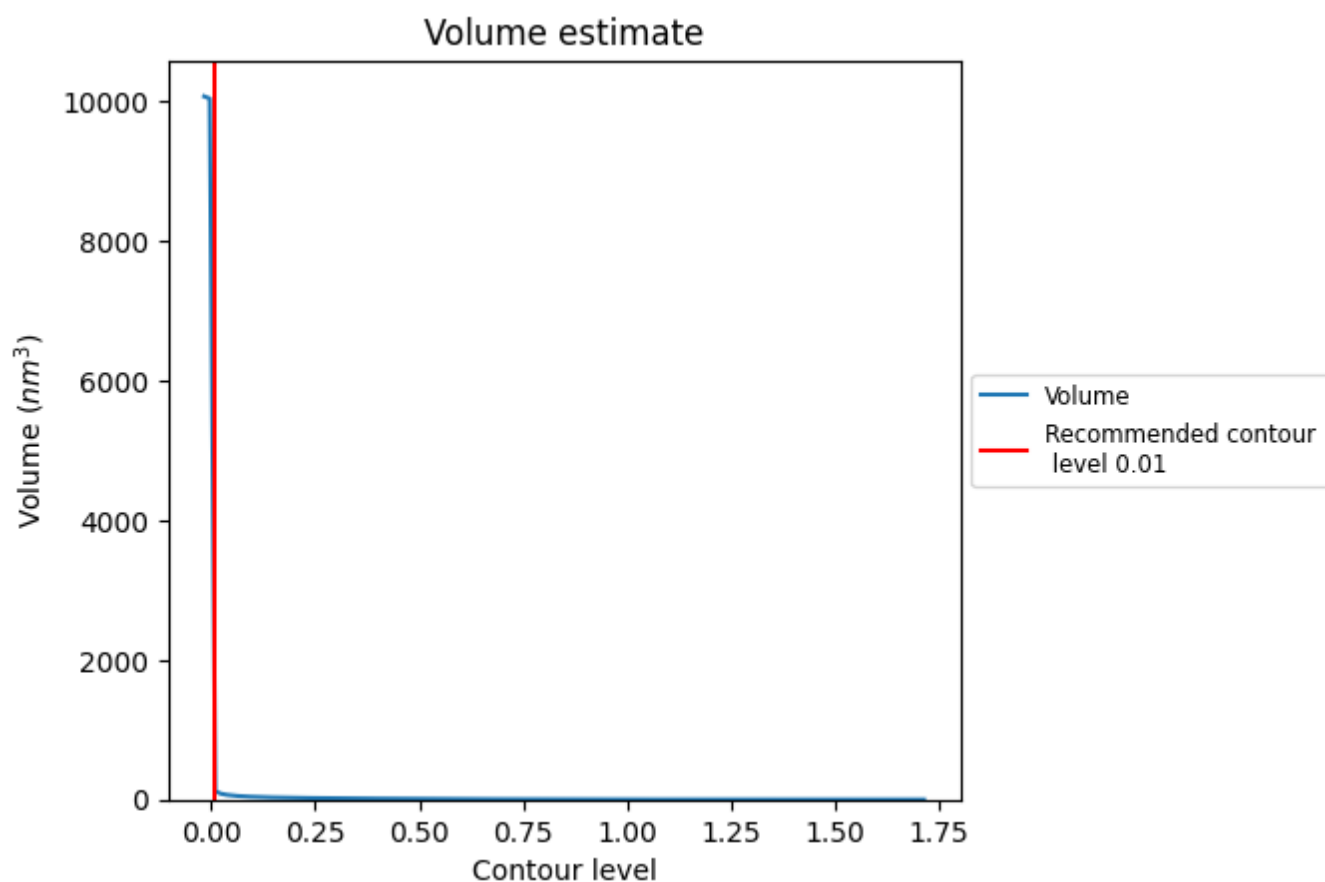
This section contains the results of statistical analysis of the map.

### 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.

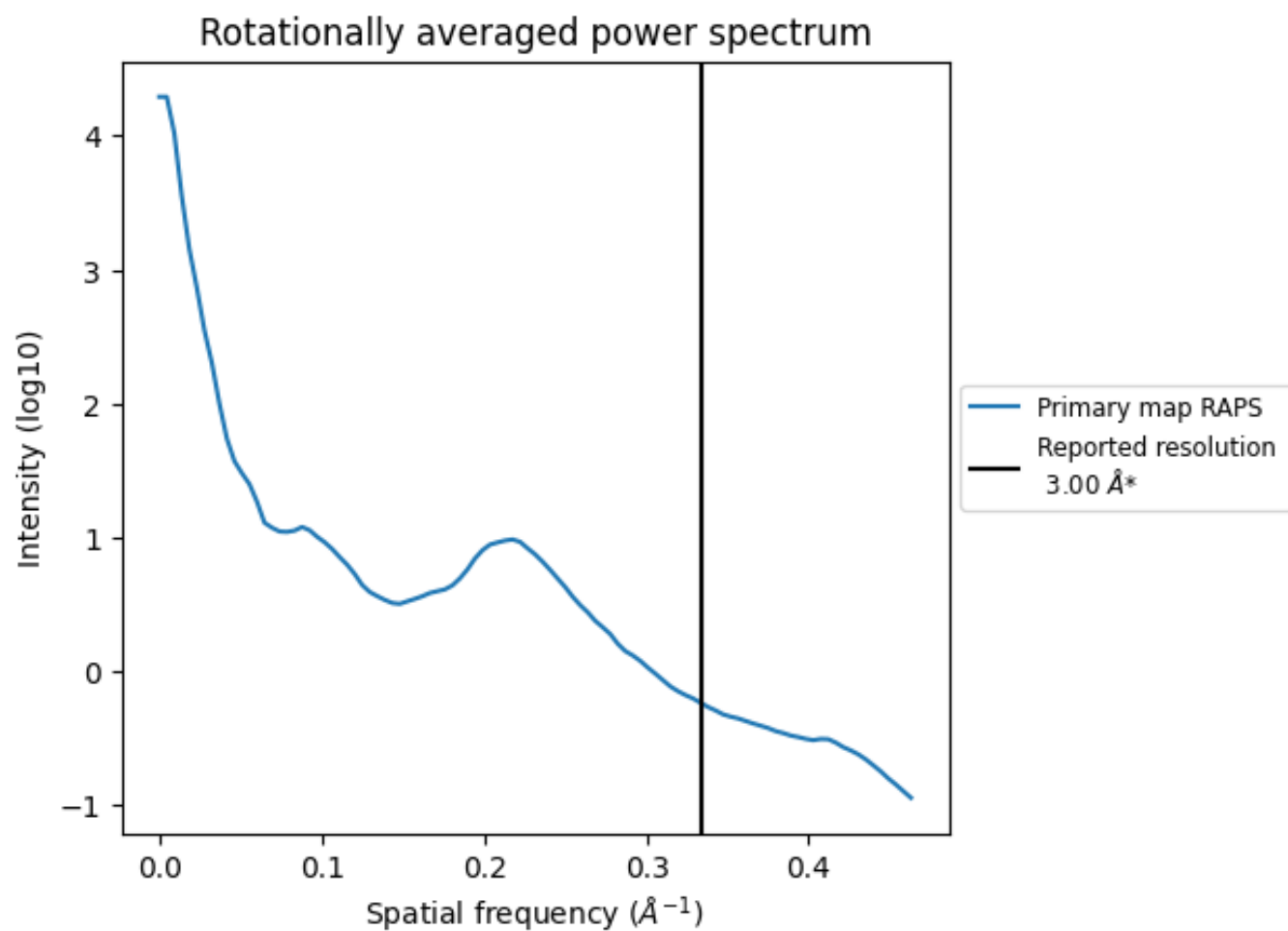
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 118 nm<sup>3</sup>; this corresponds to an approximate mass of 106 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 0.333 Å<sup>-1</sup>

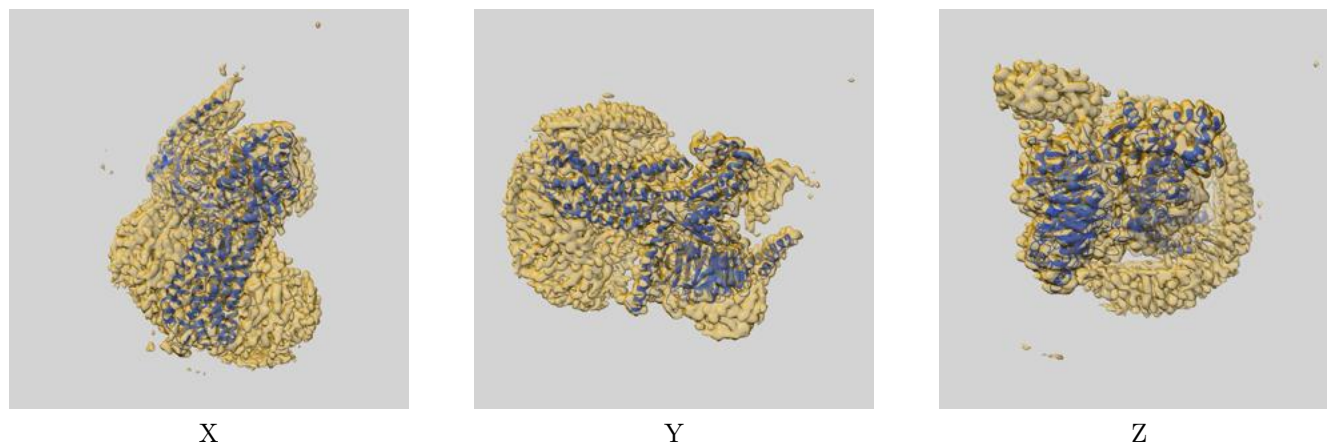
## 8 Fourier-Shell correlation ⓘ

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

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

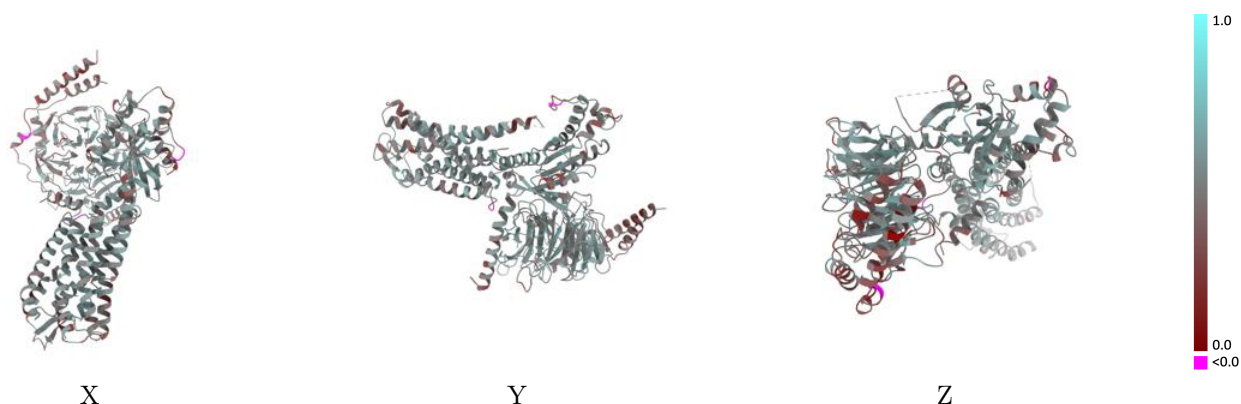
This section contains information regarding the fit between EMDB map EMD-31145 and PDB model 7EIB. Per-residue inclusion information can be found in [section 3](#) on [page 12](#).

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



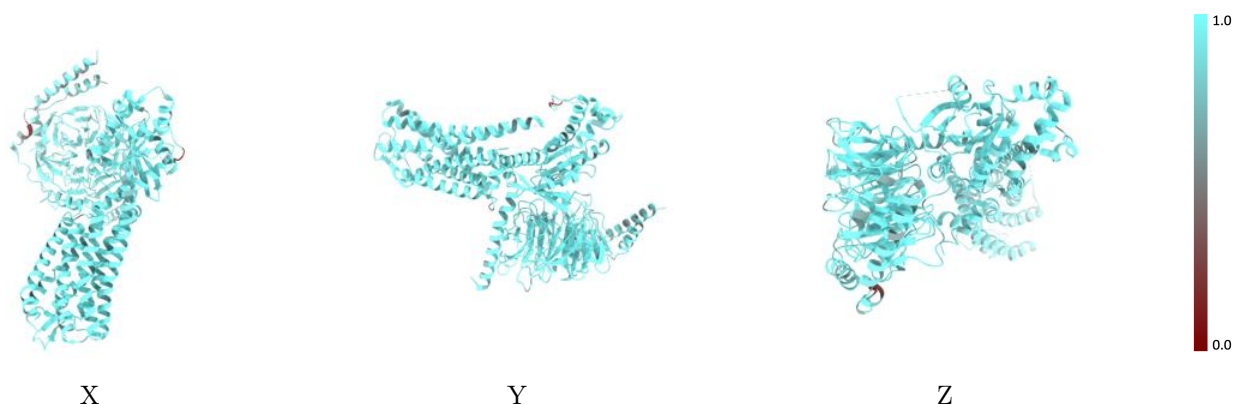
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



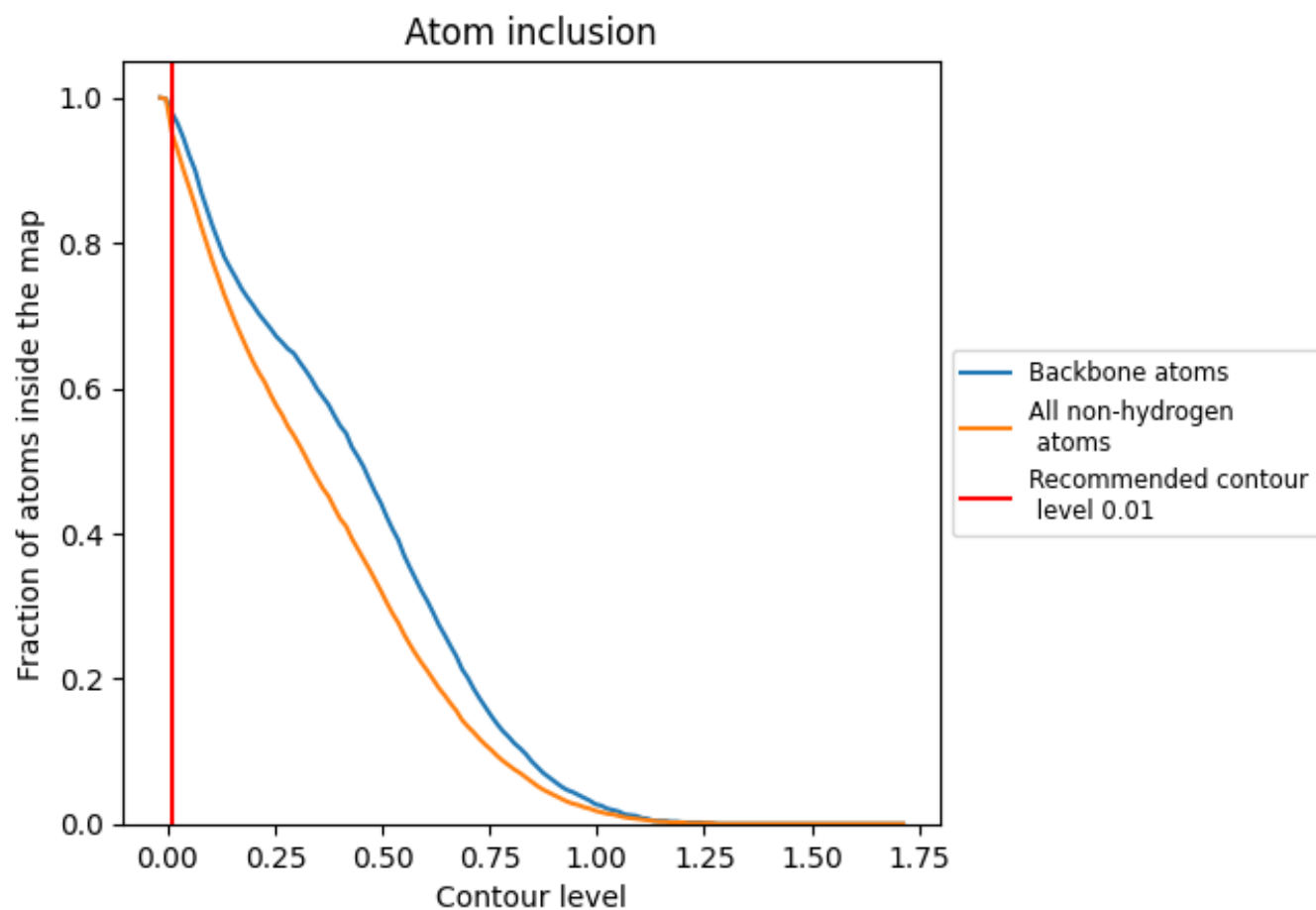
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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, 98% of all backbone atoms, 95% 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> 0.9510	<div></div> 0.4810
A	<div></div> 0.9590	<div></div> 0.4870
B	<div></div> 0.9470	<div></div> 0.4890
C	<div></div> 0.9540	<div></div> 0.4790
D	<div></div> 0.9860	<div></div> 0.5560
E	<div></div> 0.8910	<div></div> 0.3980

