



Full wwPDB EM Validation Report ⓘ

Nov 22, 2022 – 02:20 PM 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 Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

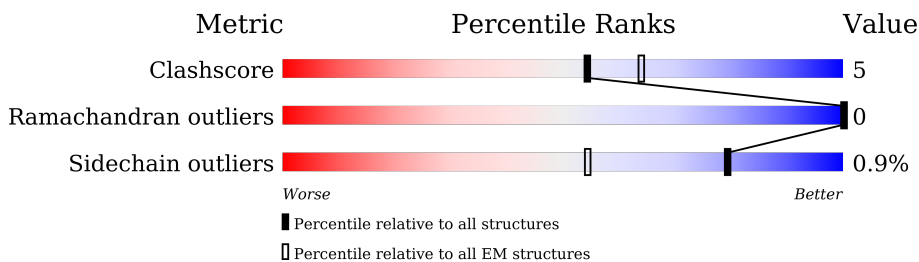
EMDB validation analysis : 0.0.1.dev43
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	
2	B	377	
3	D	9	
4	R	595	
5	S	248	
6	Y	71	

2 Entry composition i

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
			Total	C	N	O	S		
1	A	230	1878	1186	334	350	8	0	0

- 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
			Total	C	N	O	S		
2	B	341	2605	1607	469	508	21	0	0

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
			Total	C	N	O		
3	D	9	76	50	15	11	0	0

- Molecule 4 is a protein called B2 bradykinin receptor.

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

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
			Total	C	N	O	S		
5	S	232	1784	1132	295	347	10	0	0

- 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
			Total	C	N	O	S		
6	Y	51	353	222	60	69	2	0	0

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 (\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 (\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.

All (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
1:A:210:LYS:HE2	2:B:188:MET:HG3	1.82	0.62
1:A:208:ARG:NH2	1:A:239:ASP:OD1	2.26	0.61
2:B:250:CYS:HB2	2:B:264:TYR:HB2	1.83	0.59
2:B:249:THR:HG22	2:B:265:SER:HB3	1.84	0.59
2:B:221:THR:N	6:Y:22:GLU:OE1	2.35	0.58
2:B:228:ASP:N	2:B:228:ASP:OD1	2.37	0.58
2:B:294:CYS:HB3	2:B:308:LEU:HB2	1.85	0.57
1:A:282:PHE:O	1:A:303:ARG:NH2	2.38	0.56
2:B:51:LEU:HD12	2:B:336:LEU:HD23	1.86	0.56
2:B:166:CYS:HB2	2:B:180:PHE:HB2	1.86	0.56
5:S:187:LEU:HD21	5:S:190:TYR:HB3	1.88	0.55
3:D:8:PHE:CD1	4:R:141:LEU:HD11	2.42	0.55
2:B:79:LEU:HG	2:B:95:LEU:HD21	1.87	0.55
4:R:136:ILE:O	4:R:140:ASN:ND2	2.39	0.55
4:R:157:LEU:HB3	4:R:165:MET:HG3	1.89	0.54
4:R:154:ASP:OD1	4:R:169:ARG:NH2	2.39	0.54
3:D:8:PHE:HZ	4:R:322:TYR:CD1	2.25	0.54
4:R:119:ASN:HB3	4:R:122:ASP:HB3	1.89	0.53
2:B:294:CYS:O	2:B:308:LEU:N	2.36	0.53
1:A:191:VAL:O	1:A:194:VAL:HG22	2.08	0.53
4:R:271:LEU:HD21	4:R:335:VAL:HG21	1.91	0.52
5:S:100:ILE:HG23	5:S:105:SER:HB2	1.91	0.52
1:A:205:ARG:NH1	1:A:206:ASP:OD1	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:259:ASN:HA	1:A:331:THR:O	2.10	0.52
1:A:334:VAL:HG22	1:A:334:VAL:O	2.09	0.52
2:B:90:VAL:HG12	2:B:91:HIS:CE1	2.45	0.52
3:D:9:ARG:HD2	4:R:290:THR:OG1	2.11	0.51
1:A:37:LEU:HD23	1:A:221:ILE:HD12	1.94	0.50
1:A:205:ARG:NE	2:B:186:ASP:OD1	2.25	0.50
1:A:9:ASP:OD2	5:S:169:ASN:ND2	2.40	0.49
2:B:123:ILE:O	2:B:136:SER:N	2.40	0.49
3:D:8:PHE:CE1	4:R:141:LEU:HD11	2.47	0.49
5:S:52:SER:O	5:S:72:ARG:NH1	2.45	0.49
4:R:248:MET:HG2	4:R:269:THR:HG23	1.95	0.49
4:R:330:LEU:HD22	4:R:334:ILE:HB	1.95	0.48
5:S:29:PHE:O	5:S:72:ARG:NH2	2.46	0.48
1:A:194:VAL:HG11	4:R:163:MET:HB3	1.96	0.48
2:B:298:ASP:HB3	2:B:301:LYS:HB2	1.96	0.48
1:A:298:ASP:O	1:A:301:VAL:HG12	2.13	0.48
4:R:289:SER:OG	4:R:313:ILE:HG22	2.15	0.47
5:S:40:ALA:HB3	5:S:43:LYS:HB2	1.98	0.46
5:S:33:GLY:O	5:S:99:SER:N	2.45	0.46
2:B:121:CYS:HB3	2:B:139:LEU:HD12	1.98	0.46
2:B:286:LEU:HD22	2:B:327:VAL:HG11	1.98	0.45
4:R:90:THR:O	4:R:94:ILE:N	2.48	0.45
4:R:101:ALA:O	4:R:105:ILE:HG12	2.16	0.45
4:R:318:SER:O	4:R:322:TYR:HD1	1.99	0.45
2:B:51:LEU:HB2	2:B:336:LEU:HB3	1.99	0.45
2:B:186:ASP:OD1	2:B:186:ASP:N	2.49	0.45
2:B:158:VAL:HA	2:B:168:LEU:HA	1.99	0.45
2:B:198:LEU:HB3	2:B:210:LEU:HD11	1.99	0.45
2:B:81:ILE:O	2:B:90:VAL:N	2.50	0.45
1:A:34:LEU:HB3	1:A:219:THR:HG21	1.99	0.44
4:R:125:PHE:HB3	4:R:129:LEU:HD22	2.00	0.44
1:A:244:TRP:CD1	1:A:319:SER:HB2	2.52	0.44
1:A:348:ASP:O	1:A:352:GLN:HG2	2.18	0.44
3:D:8:PHE:CD1	4:R:141:LEU:HD21	2.53	0.44
4:R:158:ALA:O	4:R:162:THR:OG1	2.28	0.44
4:R:285:PRO:O	4:R:288:ILE:HG22	2.18	0.44
1:A:40:GLY:HA3	1:A:224:VAL:HG22	2.00	0.44
2:B:162:GLY:HA2	2:B:186:ASP:HB3	1.99	0.44
4:R:150:LEU:HA	4:R:153:ILE:HG22	1.99	0.44
1:A:355:LEU:HB3	1:A:361:VAL:HG23	2.00	0.43
4:R:75:ASN:HB3	4:R:104:LEU:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:CYS:HB3	2:B:139:LEU:HB2	1.99	0.43
2:B:159:THR:OG1	2:B:169:TRP:NE1	2.50	0.43
4:R:71:ALA:HB2	4:R:326:CYS:SG	2.59	0.42
4:R:107:ALA:HA	4:R:110:LEU:HD12	2.00	0.42
5:S:202:ARG:NH1	5:S:223:ASP:OD2	2.51	0.42
2:B:198:LEU:HD23	2:B:212:ASP:HA	2.01	0.42
3:D:3:PRO:HG3	4:R:297:ARG:HH11	1.85	0.42
2:B:164:THR:HG22	2:B:164:THR:O	2.20	0.42
2:B:170:ASP:OD1	2:B:171:ILE:N	2.53	0.42
4:R:183:GLY:O	4:R:187:LEU:HG	2.19	0.42
4:R:153:ILE:O	4:R:157:LEU:HG	2.20	0.42
5:S:83:MET:SD	5:S:86:LEU:HD21	2.60	0.42
4:R:233:PHE:HB2	4:R:287:GLN:NE2	2.35	0.41
1:A:48:THR:CG2	1:A:333:SER:OG	2.57	0.41
4:R:271:LEU:O	4:R:275:VAL:HG13	2.21	0.41
3:D:7:PRO:HA	4:R:113:TRP:CZ2	2.55	0.41
5:S:61:ALA:O	5:S:65:LYS:N	2.53	0.41
1:A:38:LEU:HD21	1:A:46:LYS:HB2	2.03	0.41
2:B:254:ASP:HB2	2:B:261:LEU:HD11	2.02	0.41
1:A:185:PHE:HB2	1:A:200:ASP:HB3	2.03	0.41
2:B:30:LEU:HD21	2:B:300:LEU:HA	2.01	0.41
2:B:245:SER:OG	2:B:247:ASP:OD1	2.28	0.41
4:R:233:PHE:CZ	4:R:237:LEU:HD22	2.56	0.41
1:A:184:ILE:HD13	1:A:201:VAL:HA	2.03	0.41
4:R:134:ASN:ND2	4:R:211:CYS:SG	2.95	0.41
2:B:232:ILE:HG13	2:B:243:THR:HG22	2.02	0.40
2:B:281:SER:HB3	6:Y:48:ASP:HB2	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	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
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%)	65	87
2	B	280/308 (91%)	279 (100%)	1 (0%)	91	97
3	D	8/8 (100%)	8 (100%)	0	100	100
4	R	263/524 (50%)	259 (98%)	4 (2%)	65	87
5	S	196/199 (98%)	195 (100%)	1 (0%)	88	96
6	Y	31/58 (53%)	31 (100%)	0	100	100
All	All	982/1413 (70%)	973 (99%)	9 (1%)	79	93

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	ARG
1	A	324	HIS
1	A	332	CYS
2	B	186	ASP
4	R	65	TRP
4	R	218	LEU
4	R	220	TRP

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Mol	Chain	Res	Type
4	R	295	LEU
5	S	232	HIS

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 monosaccharides 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.

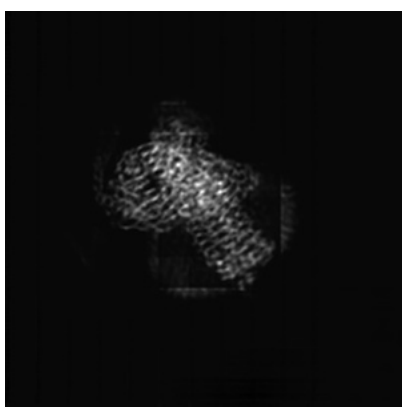
6 Map visualisation [i](#)

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.

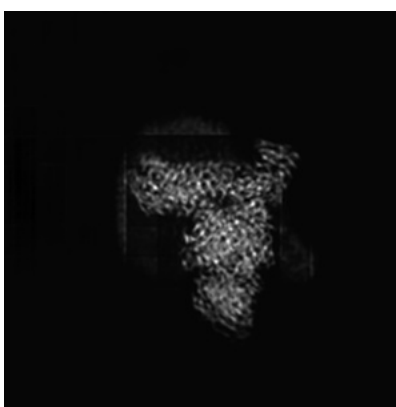
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

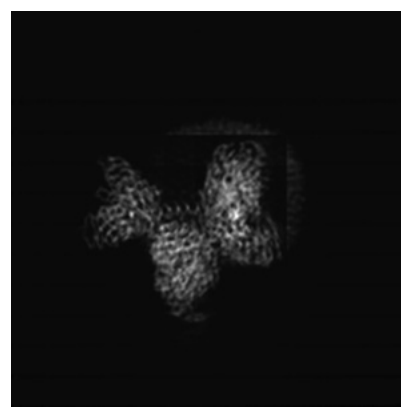
6.1.1 Primary map



X



Y

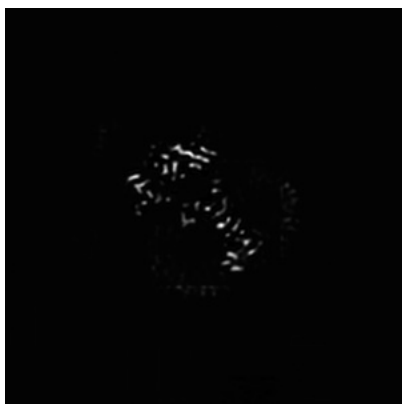


Z

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

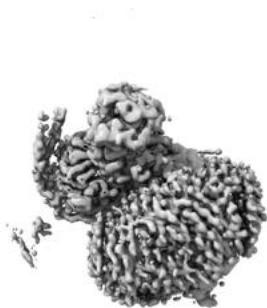


Z Index: 109

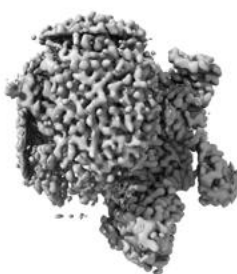
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

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.

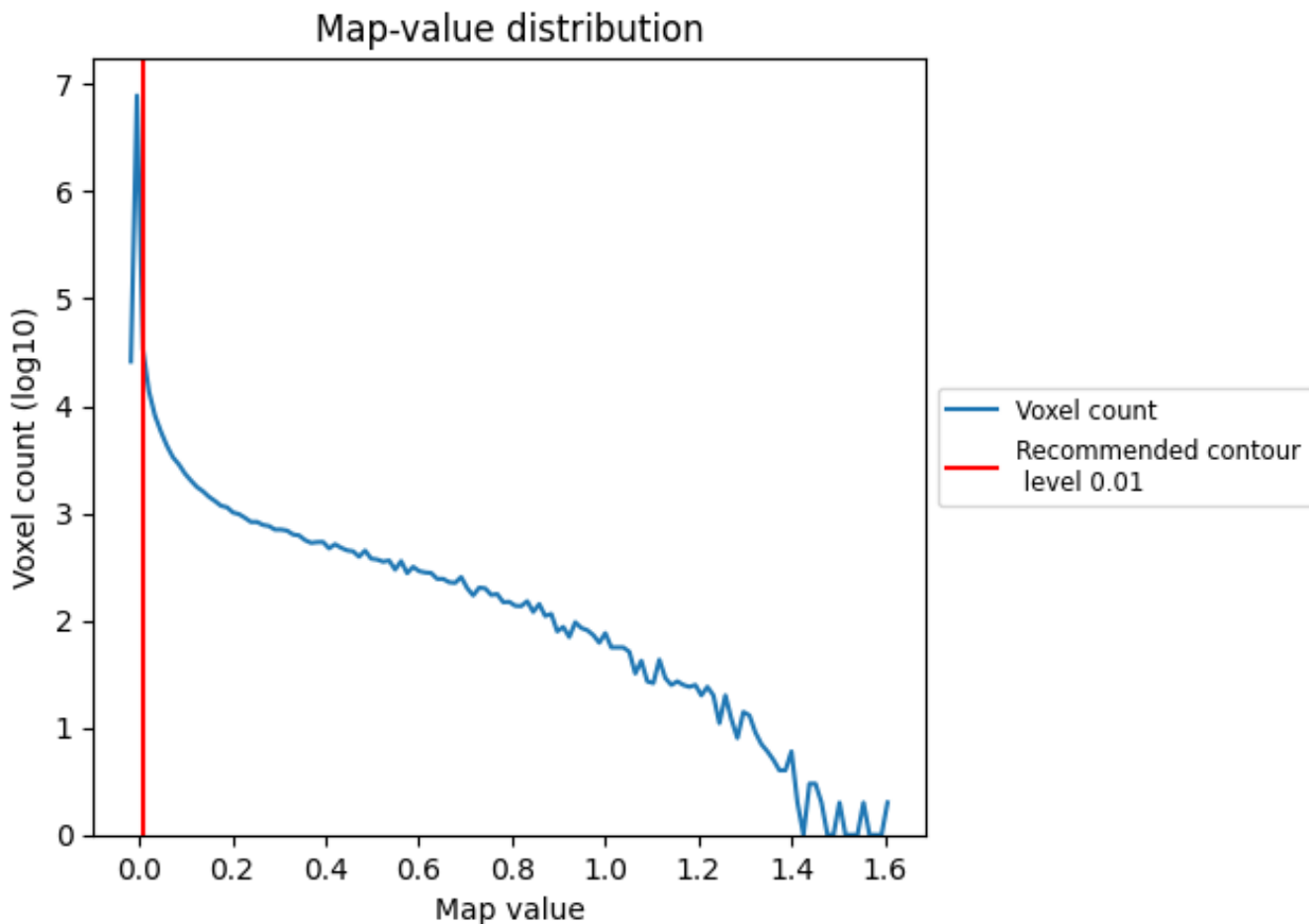
6.5 Mask visualisation

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

7 Map analysis [i](#)

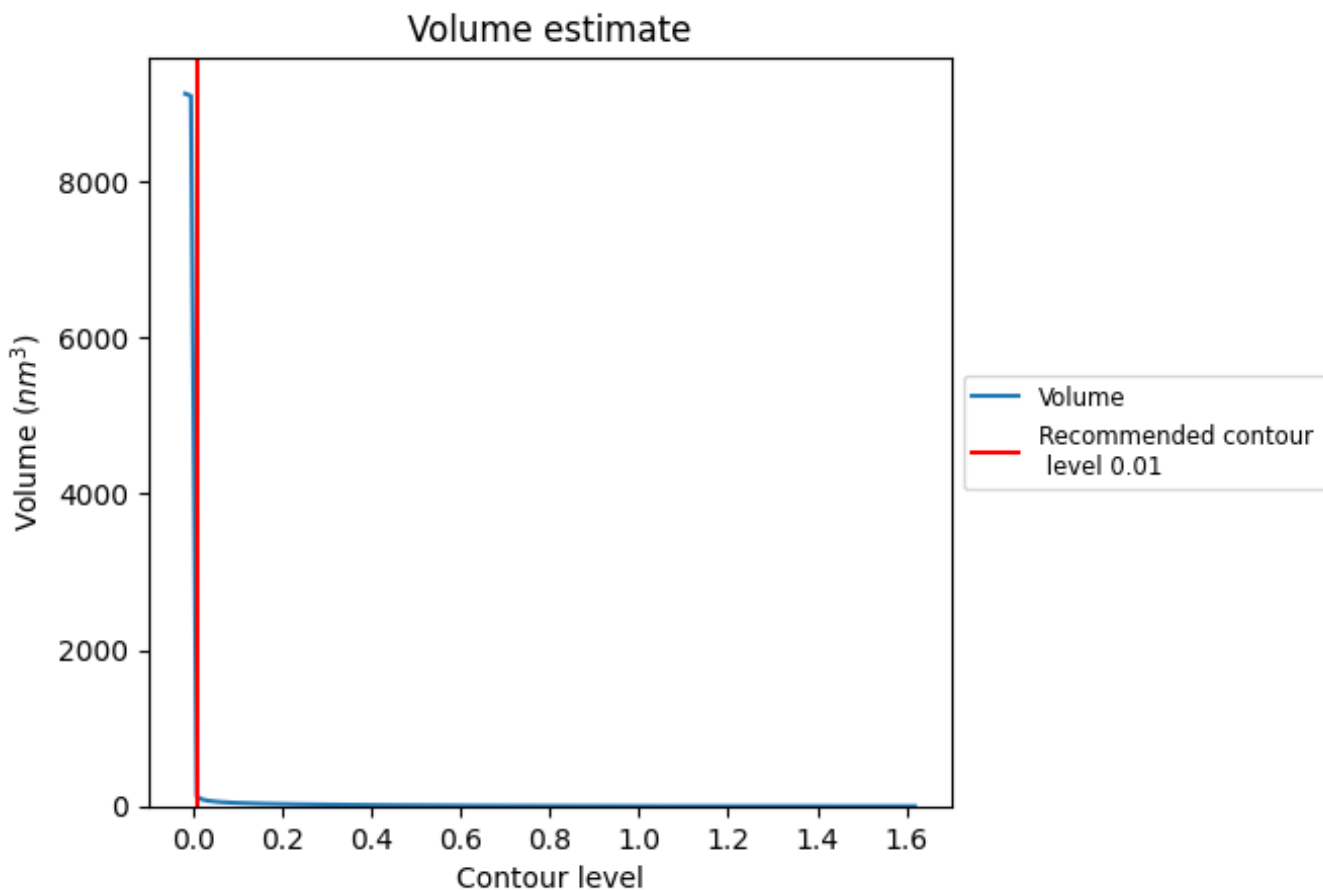
This section contains the results of statistical analysis of the map.

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.

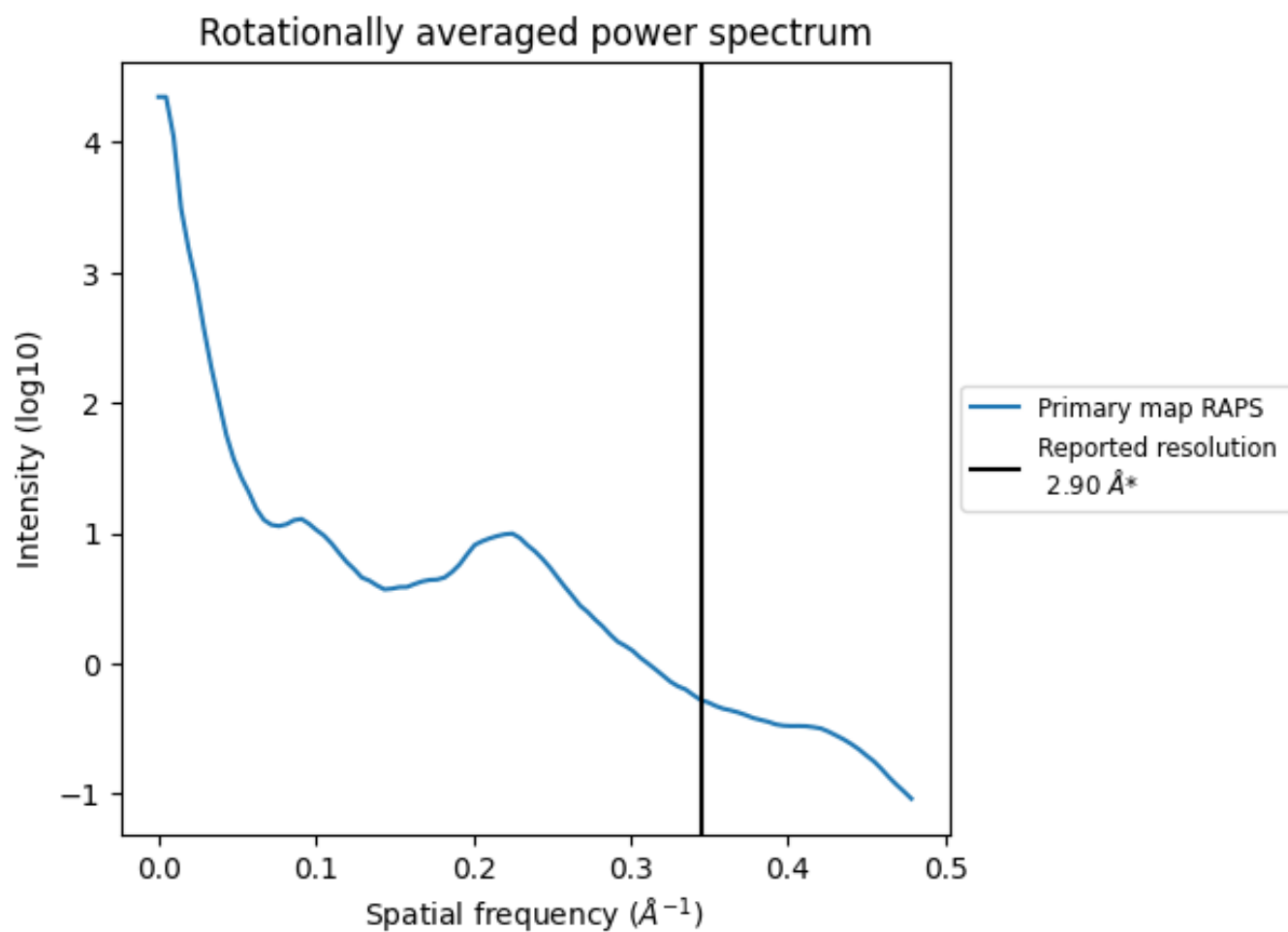
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 119 nm^3 ; 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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.345\AA^{-1}

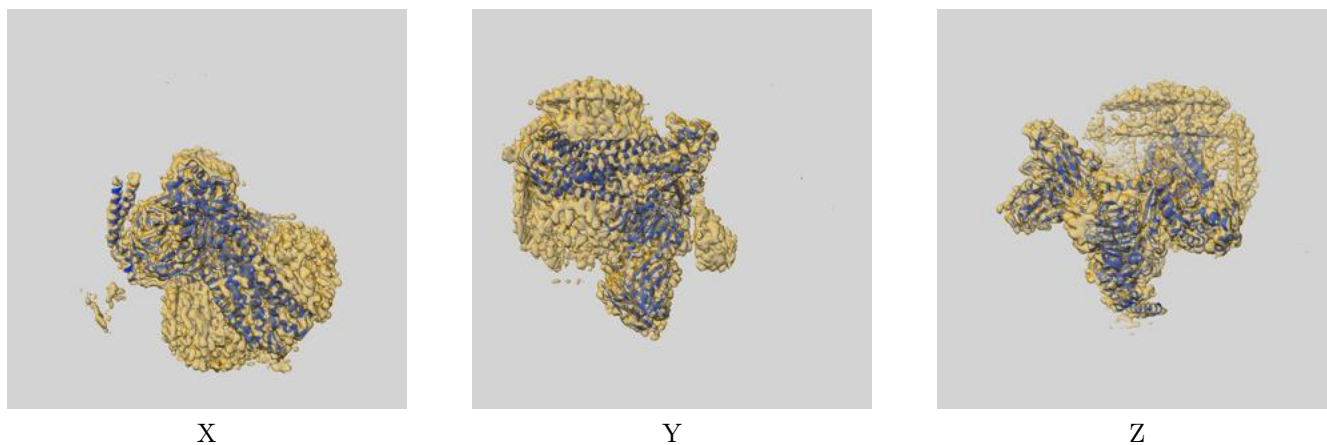
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

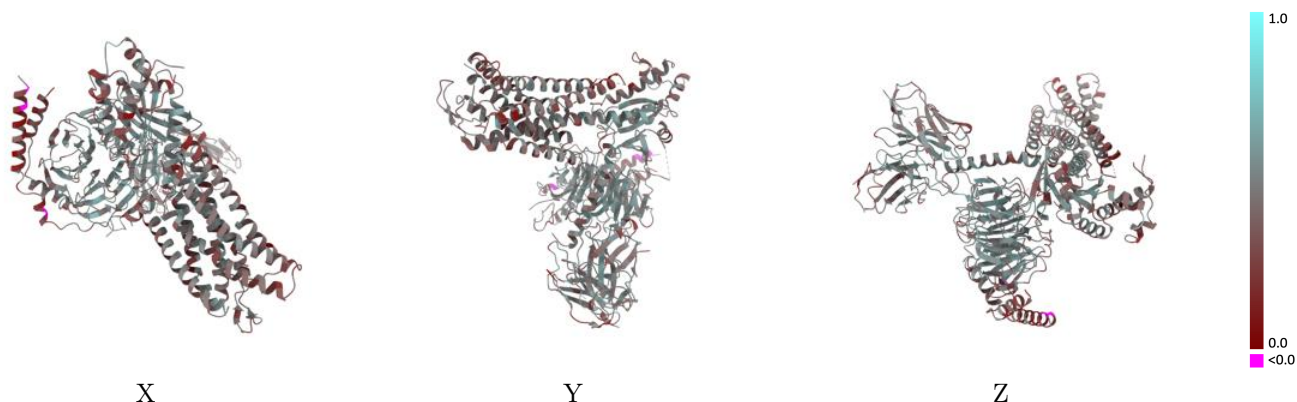
This section contains information regarding the fit between EMDB map EMD-31429 and PDB model 7F2O. Per-residue inclusion information can be found in section 3 on page 12.

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](#)



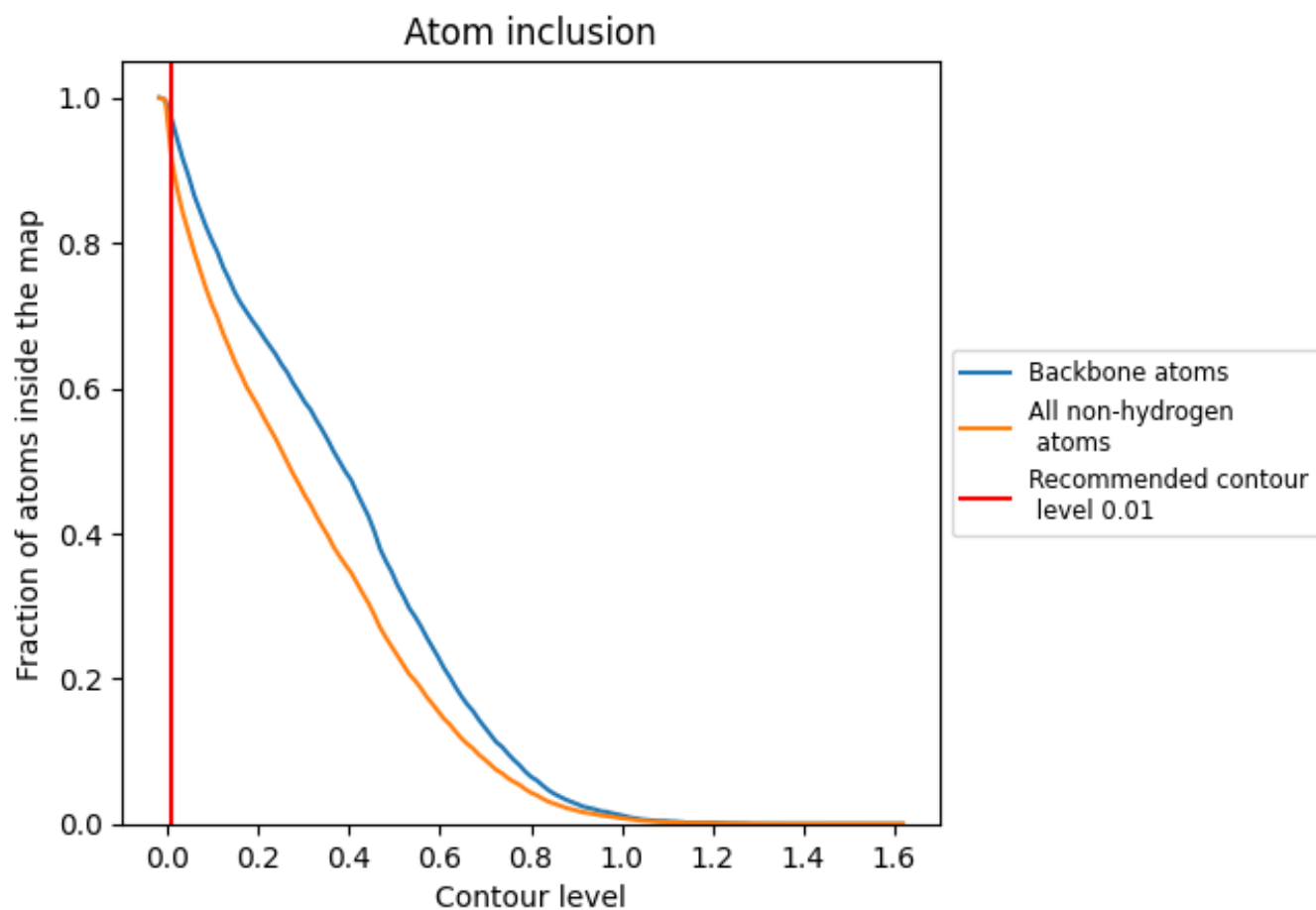
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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	 0.9115	 0.4360
A	 0.9126	 0.4510
B	 0.9139	 0.4580
D	 0.9583	 0.3770
R	 0.9134	 0.3960
S	 0.9123	 0.4520
Y	 0.8629	 0.3870

