wwPDB EM Validation Summary Report

Oct 14, 2024 – 04:49 PM JST

PDB ID	:	7VQX
EMDB ID	:	EMD-32095
Title	:	Cryo-EM structure of human vasoactive intestinal polypeptide receptor 2 (VIP2R) in complex with PACAP27 and Gs
Authors	:	Xu, Y.N.; Feng, W.B.; Zhou, Q.T.; Liang, A.Y.; Li, J.; Dai, A.T.; Zhao, F.H.; Yan, J.H.; Chen, C.W.; Li, H.; Zhao, L.H.; Xia, T.; Jiang, Y.; Xu, H.E.; Yang, D.H.; Wang, M.W.
Deposited on	:	2021-10-21
Resolution	:	2.74 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*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

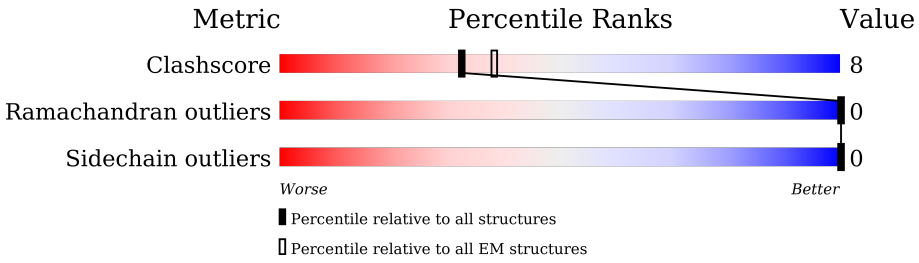
EMDB validation analysis	:	0.0.1.dev113
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.74 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 >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	394	9% 49% 11% 40%
2	B	400	10% 62% 24% 15%
3	G	71	37% 58% 20% 23%
4	L	27	15% 78% 22%
5	N	140	8% 69% 23% 9%
6	R	573	21% 51% 12% 37%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 9049 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 Guanine nucleotide-binding protein G(s) subunit alpha isoforms short.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	237	Total	C	N	O	S	0	0
			1962	1233	357	365	7		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	54	ASN	SER	engineered mutation	UNP P04896
A	226	ALA	GLY	engineered mutation	UNP P04896
A	268	ALA	GLU	engineered mutation	UNP P04896
A	271	LYS	ASN	engineered mutation	UNP P04896
A	274	ASP	LYS	engineered mutation	UNP P04896
A	280	LYS	ARG	engineered mutation	UNP P04896
A	284	ASP	THR	engineered mutation	UNP P04896
A	285	THR	ILE	engineered mutation	UNP P04896
A	366	SER	ALA	engineered mutation	UNP P04896

- 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	340	Total	C	N	O	S	0	0
			2598	1603	463	511	21		

There are 61 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-33	MET	-	initiating methionine	UNP P54311
B	-32	HIS	-	expression tag	UNP P54311
B	-31	HIS	-	expression tag	UNP P54311
B	-30	HIS	-	expression tag	UNP P54311
B	-29	HIS	-	expression tag	UNP P54311
B	-28	HIS	-	expression tag	UNP P54311

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-27	HIS	-	expression tag	UNP P54311
B	-26	SER	-	expression tag	UNP P54311
B	-25	SER	-	expression tag	UNP P54311
B	-24	GLY	-	expression tag	UNP P54311
B	-23	LEU	-	expression tag	UNP P54311
B	-22	VAL	-	expression tag	UNP P54311
B	-21	PRO	-	expression tag	UNP P54311
B	-20	ARG	-	expression tag	UNP P54311
B	-19	GLY	-	expression tag	UNP P54311
B	-18	SER	-	expression tag	UNP P54311
B	-17	HIS	-	expression tag	UNP P54311
B	-16	MET	-	expression tag	UNP P54311
B	-15	ALA	-	expression tag	UNP P54311
B	-14	SER	-	expression tag	UNP P54311
B	-13	HIS	-	expression tag	UNP P54311
B	-12	HIS	-	expression tag	UNP P54311
B	-11	HIS	-	expression tag	UNP P54311
B	-10	HIS	-	expression tag	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
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

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Chain	Residue	Modelled	Actual	Comment	Reference
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 Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	G	55	Total	C	N	O	S	0	0
			424	266	75	80	3		

- Molecule 4 is a protein called Pituitary adenylate cyclase-activating polypeptide 27.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	L	27	Total	C	N	O	S	0	0
			221	142	39	39	1		

- Molecule 5 is a protein called Nanobody-35.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	128	Total	C	N	O	S	0	0
			967	602	167	192	6		

- Molecule 6 is a protein called Vasoactive intestinal polypeptide receptor 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	R	361	Total	C	N	O	S	0	0
			2877	1889	465	501	22		

There are 158 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	439	VAL	-	expression tag	UNP P41587
R	440	PHE	-	expression tag	UNP P41587
R	441	THR	-	expression tag	UNP P41587
R	442	LEU	-	expression tag	UNP P41587
R	443	GLU	-	expression tag	UNP P41587
R	444	ASP	-	expression tag	UNP P41587
R	445	PHE	-	expression tag	UNP P41587
R	446	VAL	-	expression tag	UNP P41587
R	447	GLY	-	expression tag	UNP P41587
R	448	ASP	-	expression tag	UNP P41587
R	449	TRP	-	expression tag	UNP P41587
R	450	GLU	-	expression tag	UNP P41587
R	451	GLN	-	expression tag	UNP P41587
R	452	THR	-	expression tag	UNP P41587
R	453	ALA	-	expression tag	UNP P41587
R	454	ALA	-	expression tag	UNP P41587
R	455	TYR	-	expression tag	UNP P41587
R	456	ASN	-	expression tag	UNP P41587
R	457	LEU	-	expression tag	UNP P41587
R	458	ASP	-	expression tag	UNP P41587
R	459	GLN	-	expression tag	UNP P41587
R	460	VAL	-	expression tag	UNP P41587
R	461	LEU	-	expression tag	UNP P41587
R	462	GLU	-	expression tag	UNP P41587
R	463	GLN	-	expression tag	UNP P41587
R	464	GLY	-	expression tag	UNP P41587
R	465	GLY	-	expression tag	UNP P41587
R	466	VAL	-	expression tag	UNP P41587
R	467	SER	-	expression tag	UNP P41587
R	468	SER	-	expression tag	UNP P41587
R	469	LEU	-	expression tag	UNP P41587
R	470	LEU	-	expression tag	UNP P41587
R	471	GLN	-	expression tag	UNP P41587
R	472	ASN	-	expression tag	UNP P41587
R	473	LEU	-	expression tag	UNP P41587
R	474	ALA	-	expression tag	UNP P41587
R	475	VAL	-	expression tag	UNP P41587
R	476	SER	-	expression tag	UNP P41587
R	477	VAL	-	expression tag	UNP P41587
R	478	THR	-	expression tag	UNP P41587
R	479	PRO	-	expression tag	UNP P41587
R	480	ILE	-	expression tag	UNP P41587
R	481	GLN	-	expression tag	UNP P41587

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Chain	Residue	Modelled	Actual	Comment	Reference
R	482	ARG	-	expression tag	UNP P41587
R	483	ILE	-	expression tag	UNP P41587
R	484	VAL	-	expression tag	UNP P41587
R	485	ARG	-	expression tag	UNP P41587
R	486	SER	-	expression tag	UNP P41587
R	487	GLY	-	expression tag	UNP P41587
R	488	GLU	-	expression tag	UNP P41587
R	489	ASN	-	expression tag	UNP P41587
R	490	ALA	-	expression tag	UNP P41587
R	491	LEU	-	expression tag	UNP P41587
R	492	LYS	-	expression tag	UNP P41587
R	493	ILE	-	expression tag	UNP P41587
R	494	ASP	-	expression tag	UNP P41587
R	495	ILE	-	expression tag	UNP P41587
R	496	HIS	-	expression tag	UNP P41587
R	497	VAL	-	expression tag	UNP P41587
R	498	ILE	-	expression tag	UNP P41587
R	499	ILE	-	expression tag	UNP P41587
R	500	PRO	-	expression tag	UNP P41587
R	501	TYR	-	expression tag	UNP P41587
R	502	GLU	-	expression tag	UNP P41587
R	503	GLY	-	expression tag	UNP P41587
R	504	LEU	-	expression tag	UNP P41587
R	505	SER	-	expression tag	UNP P41587
R	506	ALA	-	expression tag	UNP P41587
R	507	ASP	-	expression tag	UNP P41587
R	508	GLN	-	expression tag	UNP P41587
R	509	MET	-	expression tag	UNP P41587
R	510	ALA	-	expression tag	UNP P41587
R	511	GLN	-	expression tag	UNP P41587
R	512	ILE	-	expression tag	UNP P41587
R	513	GLU	-	expression tag	UNP P41587
R	514	GLU	-	expression tag	UNP P41587
R	515	VAL	-	expression tag	UNP P41587
R	516	PHE	-	expression tag	UNP P41587
R	517	LYS	-	expression tag	UNP P41587
R	518	VAL	-	expression tag	UNP P41587
R	519	VAL	-	expression tag	UNP P41587
R	520	TYR	-	expression tag	UNP P41587
R	521	PRO	-	expression tag	UNP P41587
R	522	VAL	-	expression tag	UNP P41587
R	523	ASP	-	expression tag	UNP P41587

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Chain	Residue	Modelled	Actual	Comment	Reference
R	524	ASP	-	expression tag	UNP P41587
R	525	HIS	-	expression tag	UNP P41587
R	526	HIS	-	expression tag	UNP P41587
R	527	PHE	-	expression tag	UNP P41587
R	528	LYS	-	expression tag	UNP P41587
R	529	VAL	-	expression tag	UNP P41587
R	530	ILE	-	expression tag	UNP P41587
R	531	LEU	-	expression tag	UNP P41587
R	532	PRO	-	expression tag	UNP P41587
R	533	TYR	-	expression tag	UNP P41587
R	534	GLY	-	expression tag	UNP P41587
R	535	THR	-	expression tag	UNP P41587
R	536	LEU	-	expression tag	UNP P41587
R	537	VAL	-	expression tag	UNP P41587
R	538	ILE	-	expression tag	UNP P41587
R	539	ASP	-	expression tag	UNP P41587
R	540	GLY	-	expression tag	UNP P41587
R	541	VAL	-	expression tag	UNP P41587
R	542	THR	-	expression tag	UNP P41587
R	543	PRO	-	expression tag	UNP P41587
R	544	ASN	-	expression tag	UNP P41587
R	545	MET	-	expression tag	UNP P41587
R	546	LEU	-	expression tag	UNP P41587
R	547	ASN	-	expression tag	UNP P41587
R	548	TYR	-	expression tag	UNP P41587
R	549	PHE	-	expression tag	UNP P41587
R	550	GLY	-	expression tag	UNP P41587
R	551	ARG	-	expression tag	UNP P41587
R	552	PRO	-	expression tag	UNP P41587
R	553	TYR	-	expression tag	UNP P41587
R	554	GLU	-	expression tag	UNP P41587
R	555	GLY	-	expression tag	UNP P41587
R	556	ILE	-	expression tag	UNP P41587
R	557	ALA	-	expression tag	UNP P41587
R	558	VAL	-	expression tag	UNP P41587
R	559	PHE	-	expression tag	UNP P41587
R	560	ASP	-	expression tag	UNP P41587
R	561	GLY	-	expression tag	UNP P41587
R	562	LYS	-	expression tag	UNP P41587
R	563	LYS	-	expression tag	UNP P41587
R	564	ILE	-	expression tag	UNP P41587
R	565	THR	-	expression tag	UNP P41587

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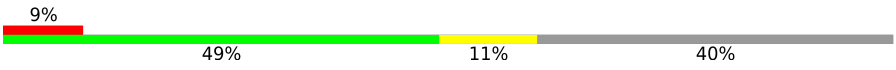
Chain	Residue	Modelled	Actual	Comment	Reference
R	566	VAL	-	expression tag	UNP P41587
R	567	THR	-	expression tag	UNP P41587
R	568	GLY	-	expression tag	UNP P41587
R	569	THR	-	expression tag	UNP P41587
R	570	LEU	-	expression tag	UNP P41587
R	571	TRP	-	expression tag	UNP P41587
R	572	ASN	-	expression tag	UNP P41587
R	573	GLY	-	expression tag	UNP P41587
R	574	ASN	-	expression tag	UNP P41587
R	575	LYS	-	expression tag	UNP P41587
R	576	ILE	-	expression tag	UNP P41587
R	577	ILE	-	expression tag	UNP P41587
R	578	ASP	-	expression tag	UNP P41587
R	579	GLU	-	expression tag	UNP P41587
R	580	ARG	-	expression tag	UNP P41587
R	581	LEU	-	expression tag	UNP P41587
R	582	ILE	-	expression tag	UNP P41587
R	583	THR	-	expression tag	UNP P41587
R	584	PRO	-	expression tag	UNP P41587
R	585	ASP	-	expression tag	UNP P41587
R	586	GLY	-	expression tag	UNP P41587
R	587	SER	-	expression tag	UNP P41587
R	588	MET	-	expression tag	UNP P41587
R	589	LEU	-	expression tag	UNP P41587
R	590	PHE	-	expression tag	UNP P41587
R	591	ARG	-	expression tag	UNP P41587
R	592	VAL	-	expression tag	UNP P41587
R	593	THR	-	expression tag	UNP P41587
R	594	ILE	-	expression tag	UNP P41587
R	595	ASN	-	expression tag	UNP P41587
R	596	SER	-	expression tag	UNP P41587

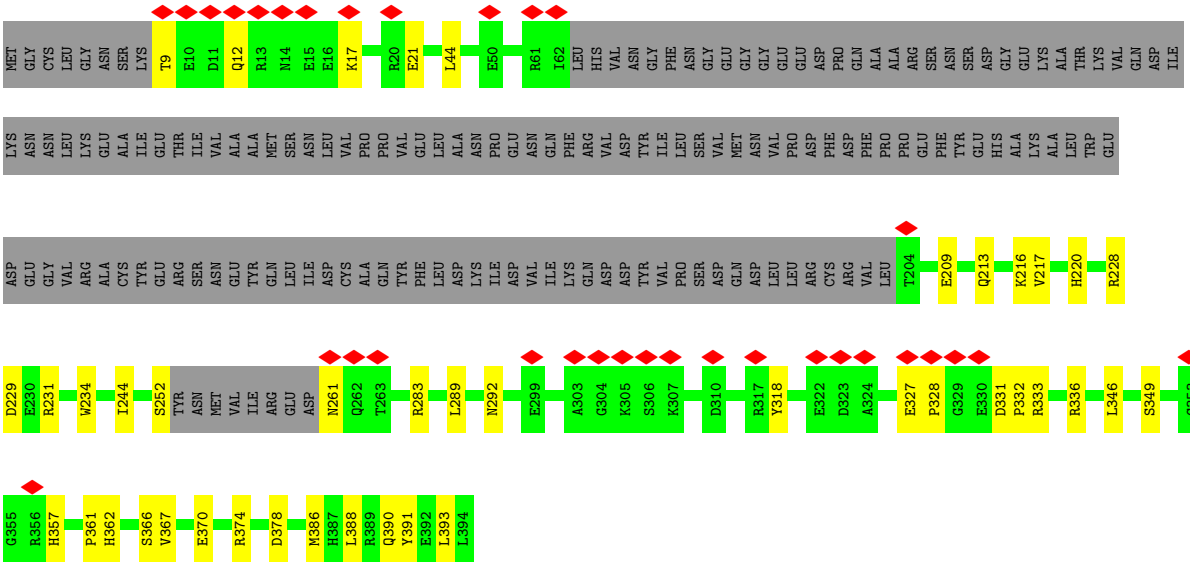
3 Residue-property plots (i)

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: Guanine nucleotide-binding protein G(s) subunit alpha isoforms short

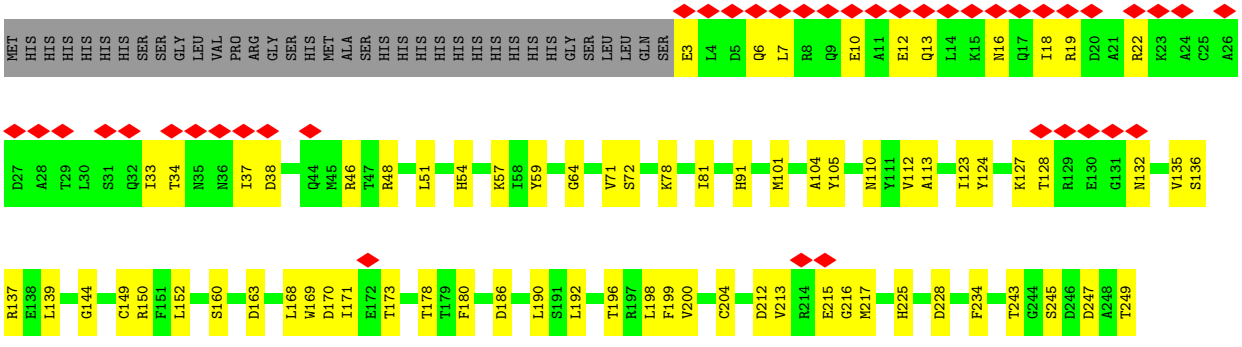
Chain A:

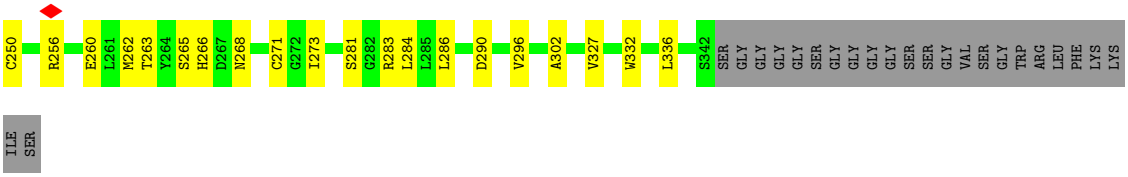




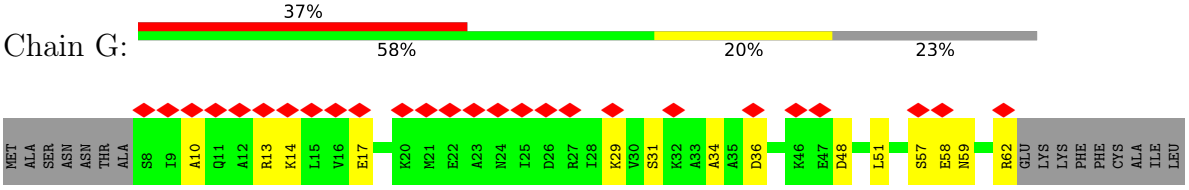
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:

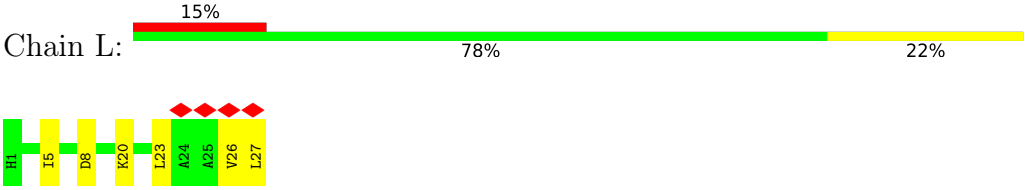




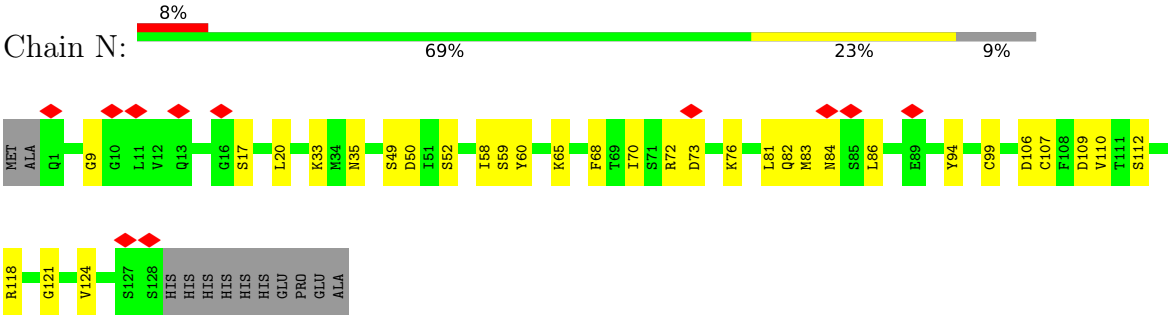
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2



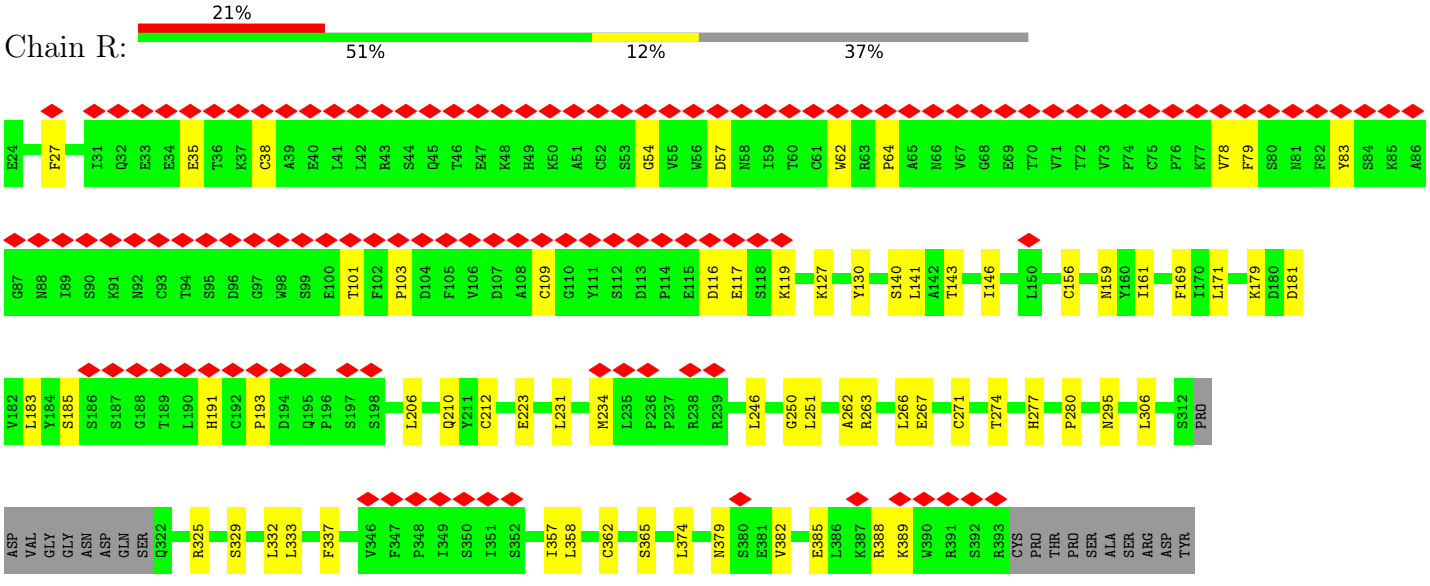
• Molecule 4: Pituitary adenylate cyclase-activating polypeptide 27

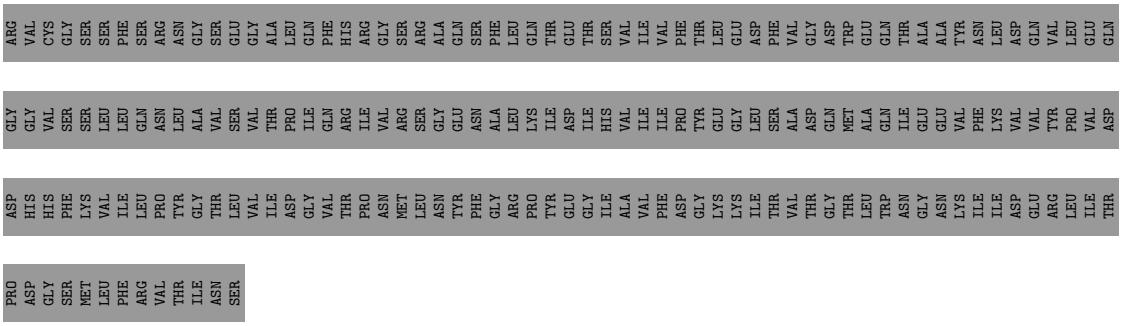


• Molecule 5: Nanobody-35



• Molecule 6: Vasoactive intestinal polypeptide receptor 2




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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	602466	Depositor
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	4.646	Depositor
Minimum map value	-2.992	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.077	Depositor
Recommended contour level	0.43	Depositor
Map size (Å)	274.176, 274.176, 274.176	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.071, 1.071, 1.071	Depositor

5 Model quality

5.1 Standard geometry

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	0/1997	0.51	0/2683
2	B	0.28	0/2645	0.55	0/3588
3	G	0.24	0/430	0.46	0/580
4	L	0.27	0/225	0.41	0/300
5	N	0.33	0/987	0.53	0/1338
6	R	0.26	0/2955	0.45	0/4025
All	All	0.28	0/9239	0.50	0/12514

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	1962	0	1943	27	0
2	B	2598	0	2491	55	0
3	G	424	0	436	10	0
4	L	221	0	226	6	0
5	N	967	0	927	21	0
6	R	2877	0	2868	41	0
All	All	9049	0	8891	148	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 8.

The worst 5 of 148 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:213:GLN:HE21	1:A:216:LYS:HA	1.50	0.76
2:B:160:SER:HB2	2:B:190:LEU:HD23	1.72	0.71
5:N:50:ASP:OD1	5:N:59:SER:OG	2.09	0.70
6:R:295:ASN:ND2	6:R:337:PHE:O	2.26	0.69
6:R:156:CYS:SG	6:R:159:ASN:ND2	2.64	0.69

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	231/394 (59%)	225 (97%)	6 (3%)	0	100	100
2	B	338/400 (84%)	326 (96%)	12 (4%)	0	100	100
3	G	53/71 (75%)	52 (98%)	1 (2%)	0	100	100
4	L	25/27 (93%)	25 (100%)	0	0	100	100
5	N	126/140 (90%)	120 (95%)	6 (5%)	0	100	100
6	R	357/573 (62%)	341 (96%)	16 (4%)	0	100	100
All	All	1130/1605 (70%)	1089 (96%)	41 (4%)	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	213/351 (61%)	213 (100%)	0	100	100
2	B	280/328 (85%)	280 (100%)	0	100	100
3	G	45/58 (78%)	45 (100%)	0	100	100
4	L	23/23 (100%)	23 (100%)	0	100	100
5	N	105/116 (90%)	105 (100%)	0	100	100
6	R	319/510 (62%)	319 (100%)	0	100	100
All	All	985/1386 (71%)	985 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	GLN
1	A	390	GLN
2	B	268	ASN
6	R	159	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.

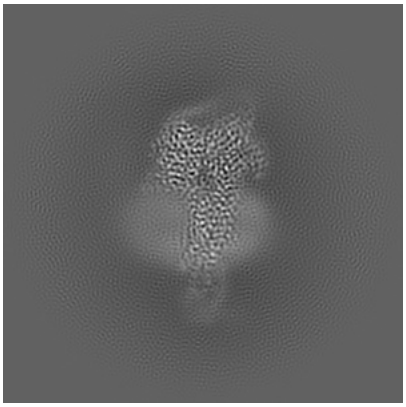
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32095. These allow visual inspection of the internal detail of the map and identification of artifacts.

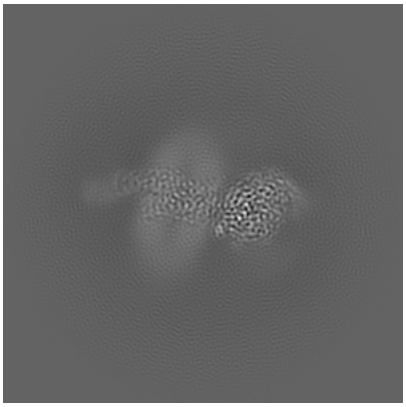
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

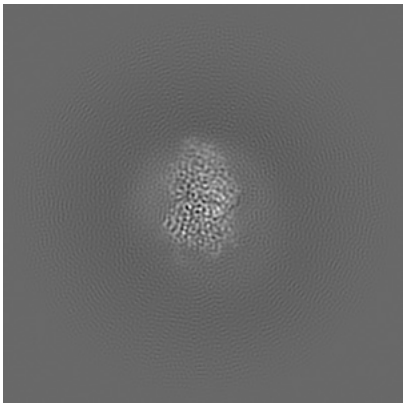
6.1.1 Primary map



X



Y

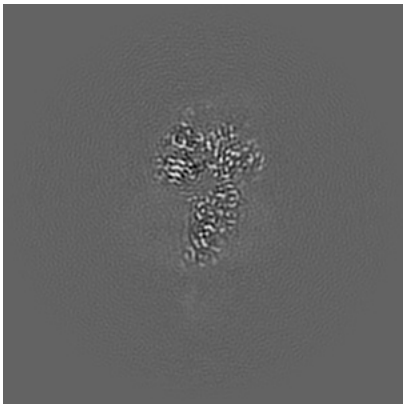


Z

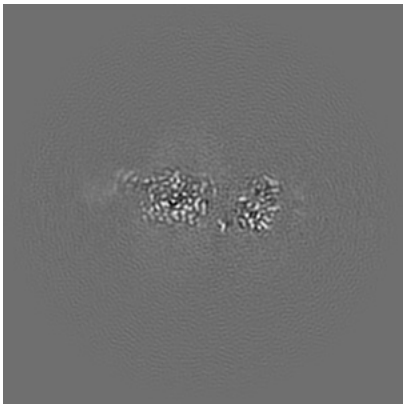
The images above show the map projected in three orthogonal directions.

6.2 Central slices

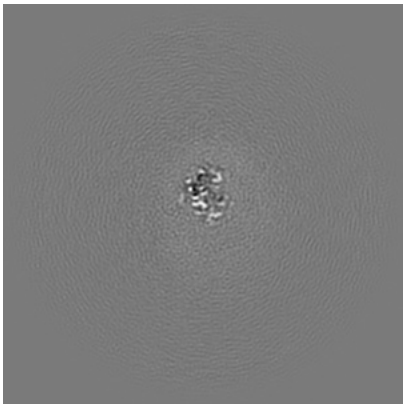
6.2.1 Primary map



X Index: 128



Y Index: 128

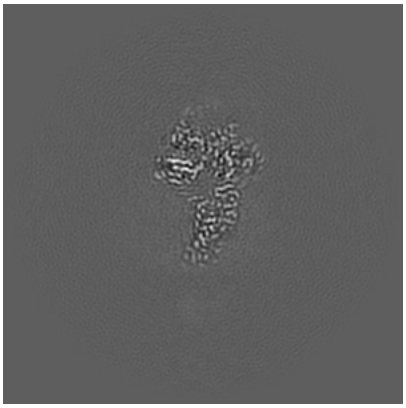


Z Index: 128

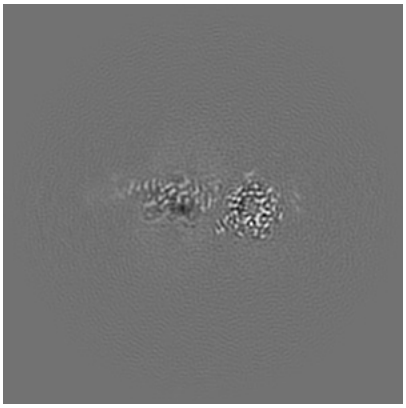
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

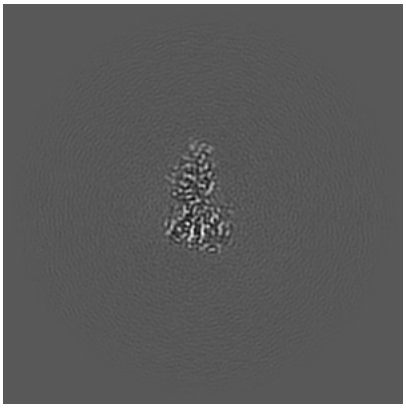
6.3.1 Primary map



X Index: 127



Y Index: 122

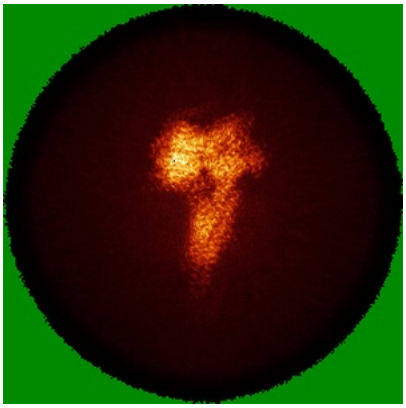


Z Index: 155

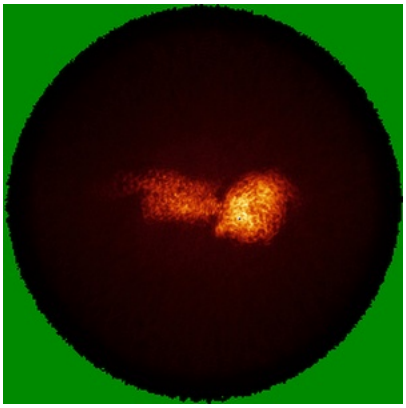
The images above show the largest variance slices of the map in three orthogonal directions.

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

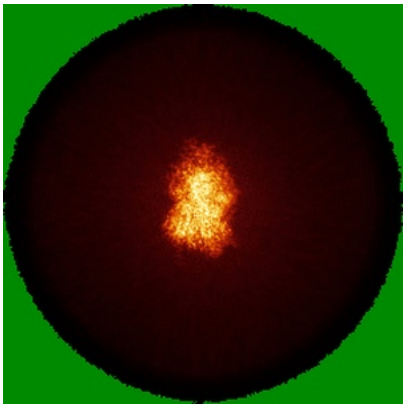
6.4.1 Primary map



X



Y

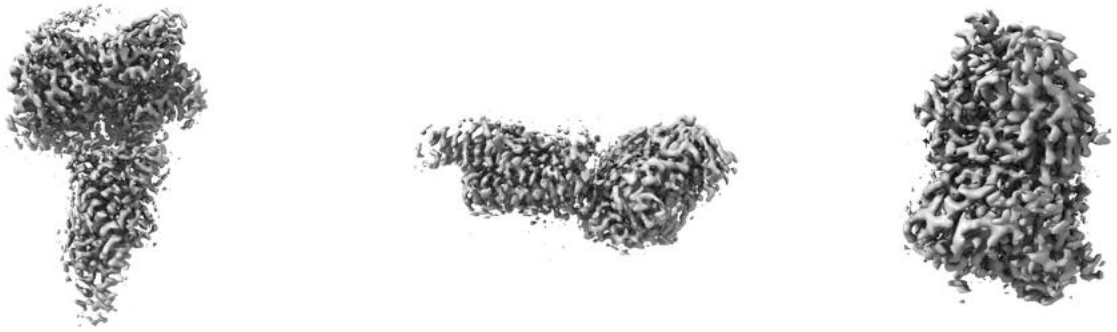


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.43. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

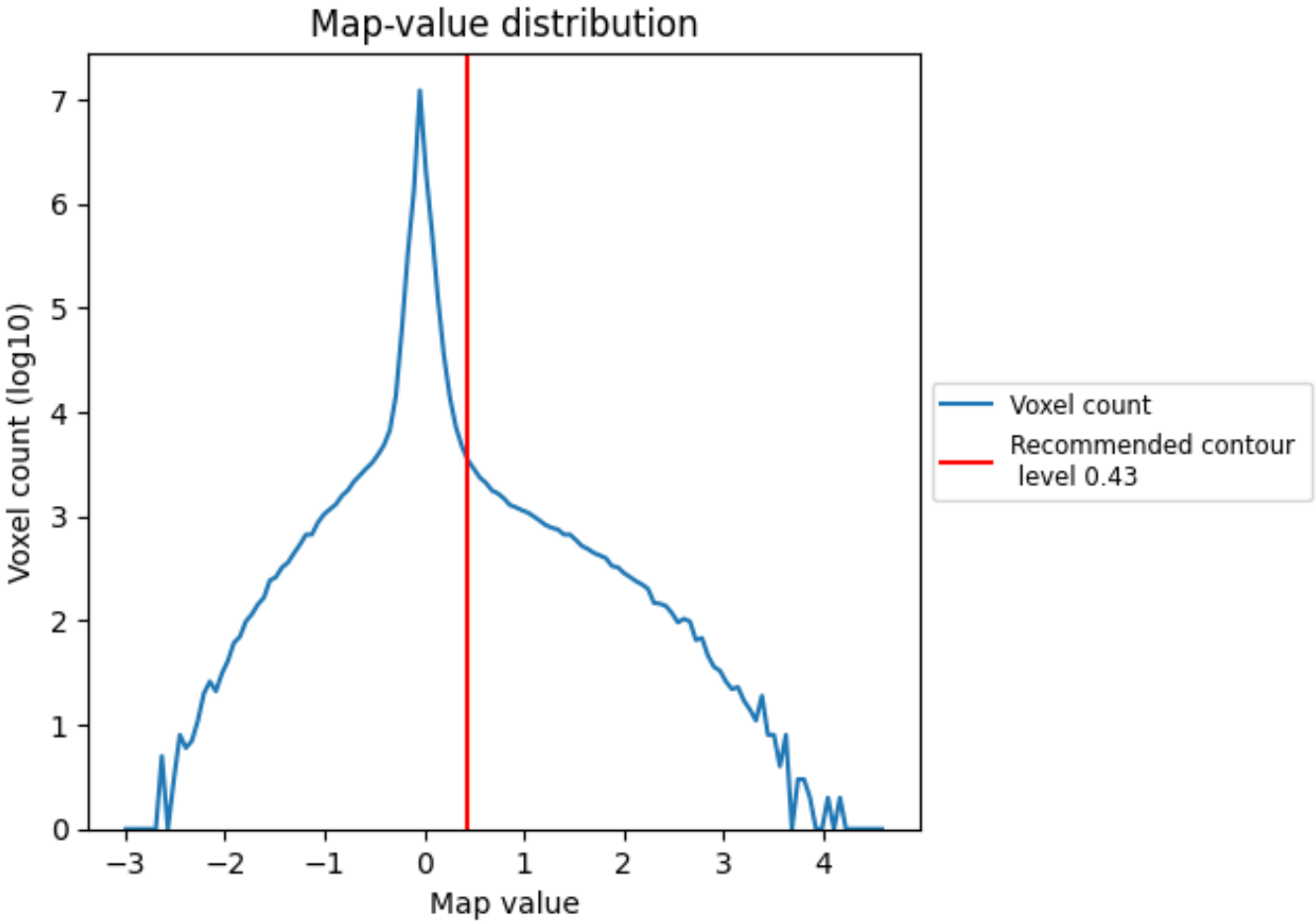
6.6 Mask visualisation (i)

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

7 Map analysis

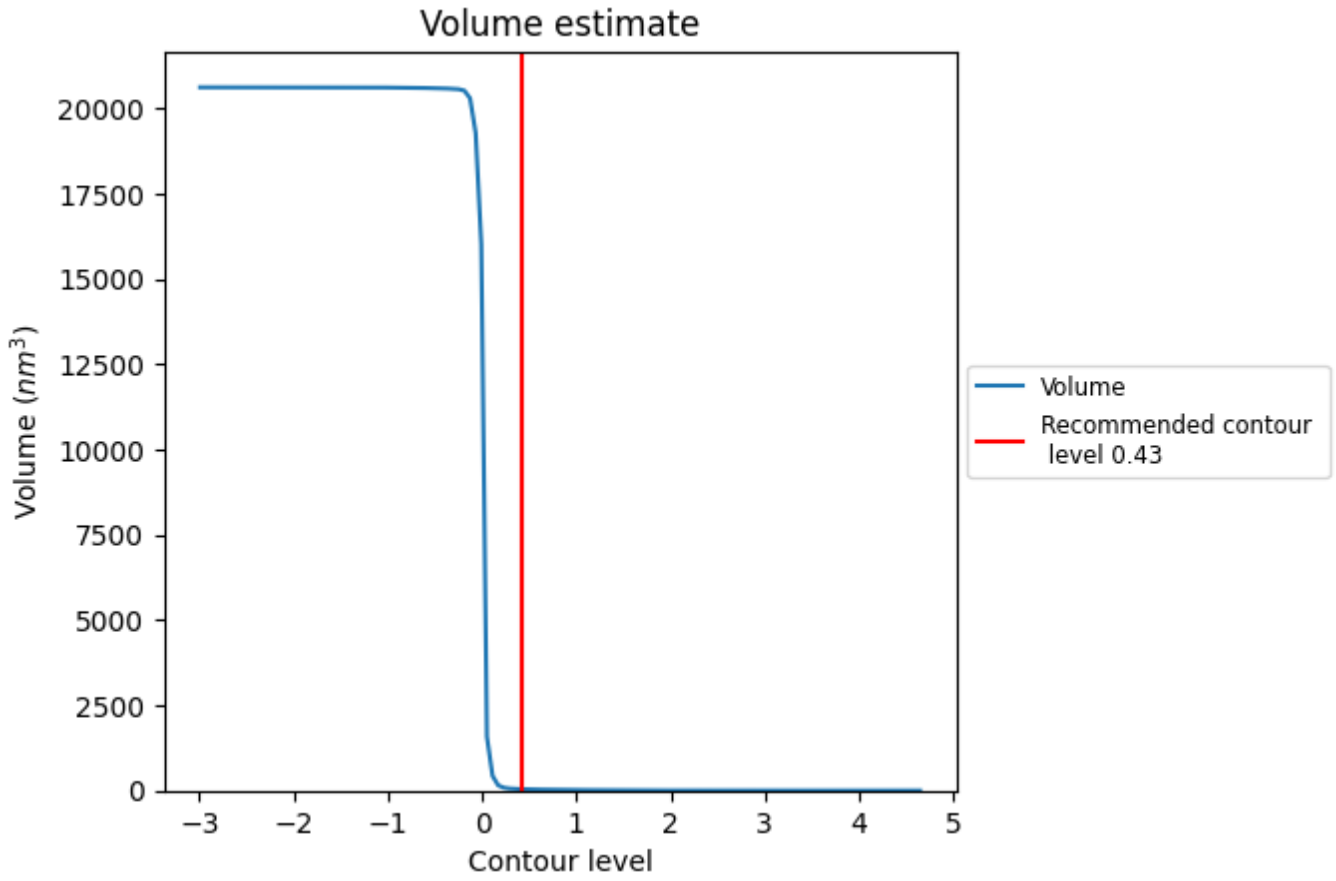
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

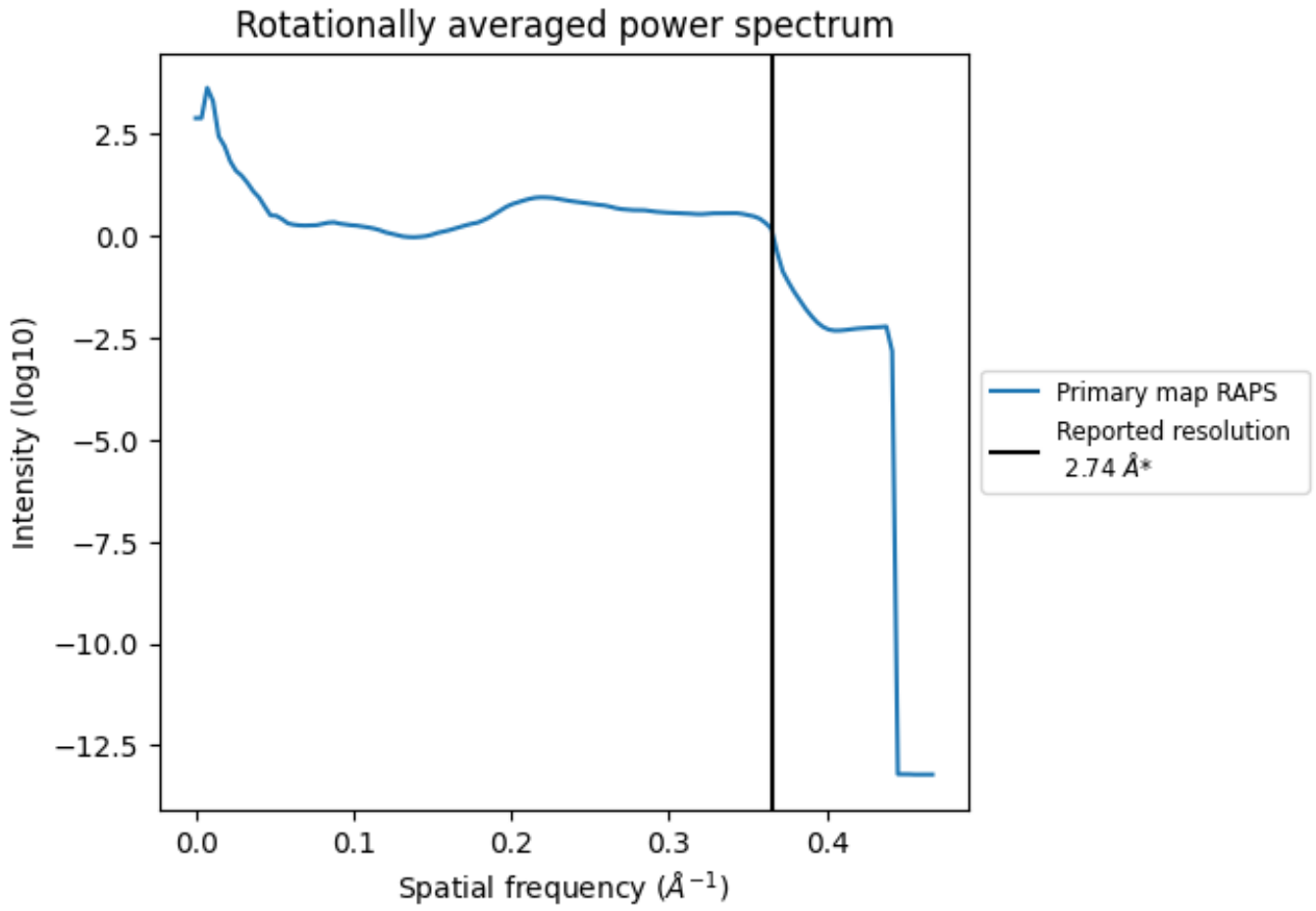
7.2 Volume estimate (i)



The volume at the recommended contour level is 40 nm^3; this corresponds to an approximate mass of 36 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 0.365 $Å^{-1}$

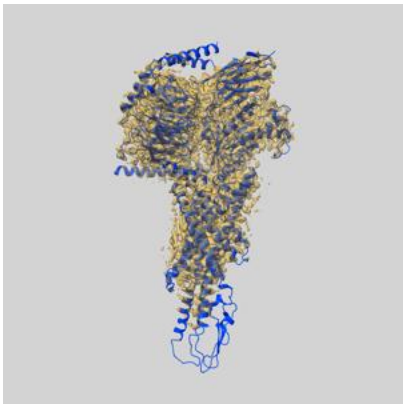
8 Fourier-Shell correlation (i)

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

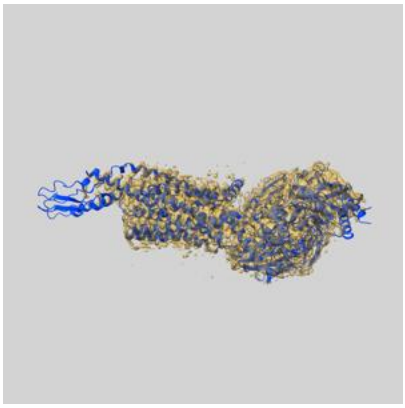
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32095 and PDB model 7VQX. Per-residue inclusion information can be found in section 3 on page 10.

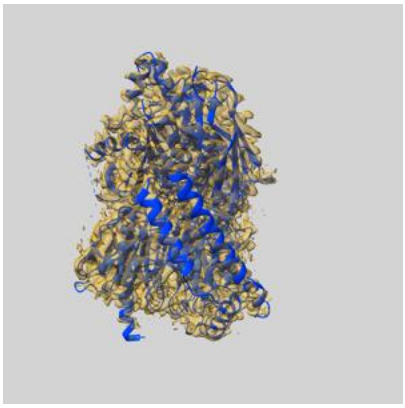
9.1 Map-model overlay



X



Y



Z

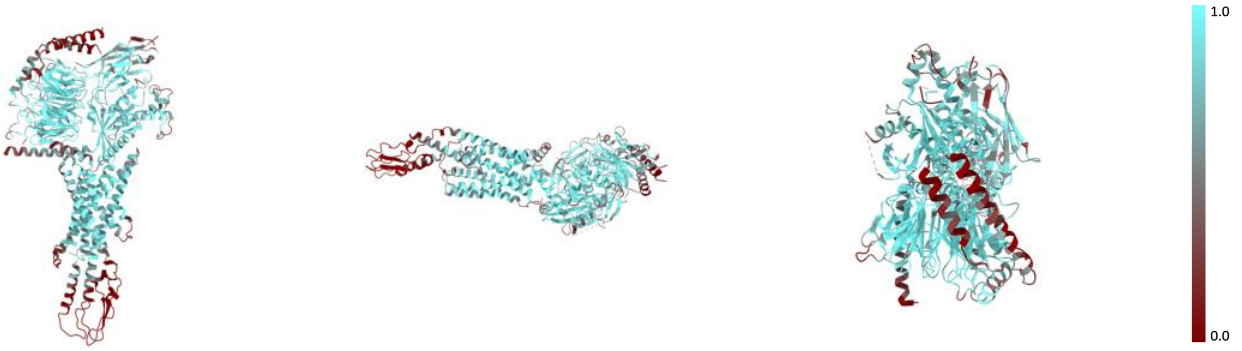
The images above show the 3D surface view of the map at the recommended contour level 0.43 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)

X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

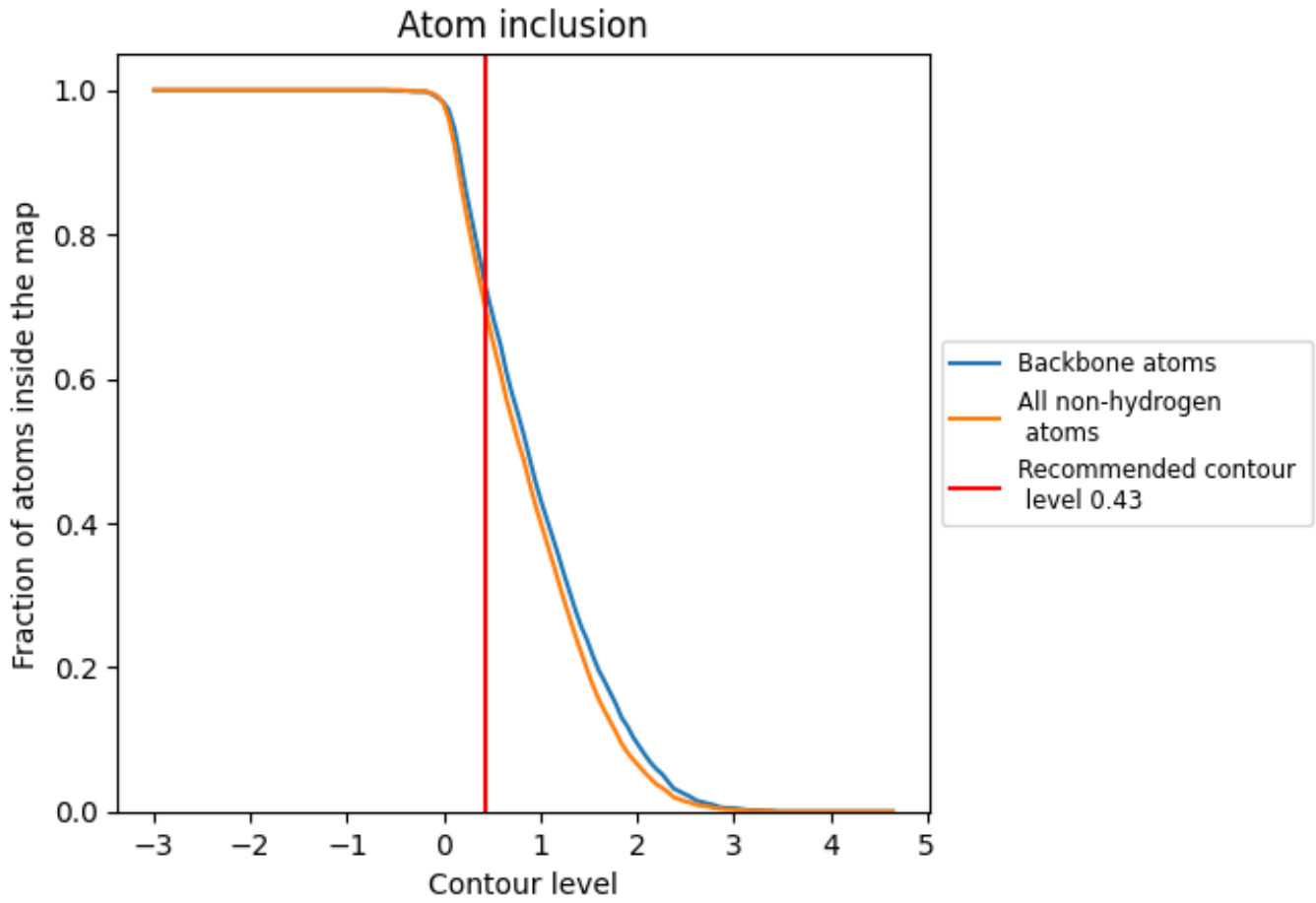
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.43).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 70% 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 (0.43) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6980	0.5430
A	0.7530	0.5740
B	0.8150	0.5940
G	0.4480	0.4790
L	0.6680	0.5510
N	0.7500	0.5770
R	0.5770	0.4730