



wwPDB EM Validation Summary Report ⓘ

Mar 9, 2026 – 10:43 AM UTC

PDB ID : 7W40 / pdb_00007w40
EMDB ID : EMD-32298
Title : Cryo-EM Structure of Human Gastrin Releasing Peptide Receptor in complex with the agonist Bombesin (6-14) [D-Phe6, beta-Ala11, Phe13, Nle14] and Gq heterotrimers
Authors : Zhan, Y.; Peng, S.; Zhang, H.
Deposited on : 2021-11-26
Resolution : 3.00 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:

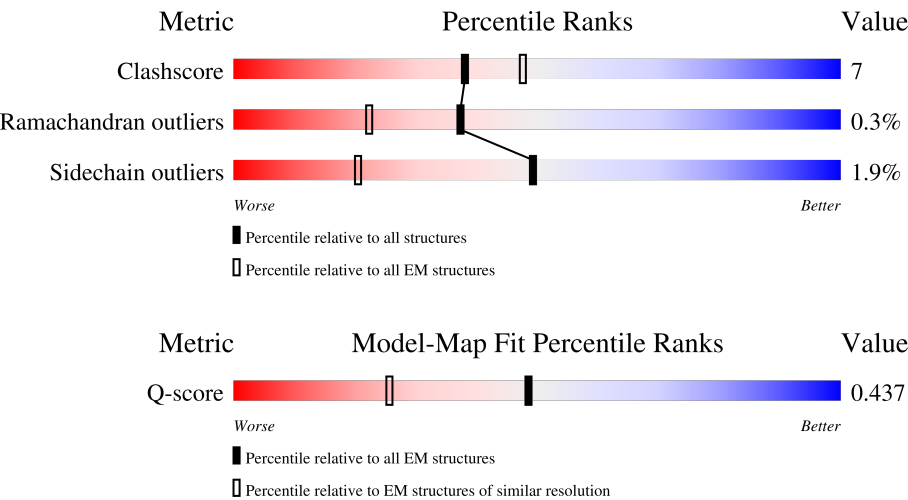
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14081 (2.50 - 3.50)

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	897	
2	B	353	
3	C	380	
4	D	81	

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Mol	Chain	Length	Quality of chain
5	H	303	9% 66% 9% 24%
6	E	9	33% 22% 56% 11% 11%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9236 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 Maltodextrin-binding protein, Gastrin-releasing peptide receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	301	2280	1503	380	384	13	0	0

There are 217 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-383	MET	-	initiating methionine	UNP A0A6D0N546
A	-382	LYS	-	expression tag	UNP A0A6D0N546
A	-381	THR	-	expression tag	UNP A0A6D0N546
A	-380	ILE	-	expression tag	UNP A0A6D0N546
A	-379	ILE	-	expression tag	UNP A0A6D0N546
A	-378	ALA	-	expression tag	UNP A0A6D0N546
A	-377	LEU	-	expression tag	UNP A0A6D0N546
A	-376	SER	-	expression tag	UNP A0A6D0N546
A	-375	TYR	-	expression tag	UNP A0A6D0N546
A	-374	ILE	-	expression tag	UNP A0A6D0N546
A	-373	PHE	-	expression tag	UNP A0A6D0N546
A	-372	CYS	-	expression tag	UNP A0A6D0N546
A	-371	LEU	-	expression tag	UNP A0A6D0N546
A	-370	VAL	-	expression tag	UNP A0A6D0N546
A	-369	PHE	-	expression tag	UNP A0A6D0N546
A	-368	ALA	-	expression tag	UNP A0A6D0N546
A	-367	ASP	-	expression tag	UNP A0A6D0N546
A	-366	TYR	-	expression tag	UNP A0A6D0N546
A	-365	LYS	-	expression tag	UNP A0A6D0N546
A	-364	ASP	-	expression tag	UNP A0A6D0N546
A	-363	ASP	-	expression tag	UNP A0A6D0N546
A	-362	ASP	-	expression tag	UNP A0A6D0N546
A	-361	ASP	-	expression tag	UNP A0A6D0N546
A	-360	LYS	-	expression tag	UNP A0A6D0N546
A	-359	HIS	-	expression tag	UNP A0A6D0N546
A	-358	HIS	-	expression tag	UNP A0A6D0N546
A	-357	HIS	-	expression tag	UNP A0A6D0N546

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-356	HIS	-	expression tag	UNP A0A6D0N546
A	-355	HIS	-	expression tag	UNP A0A6D0N546
A	-354	HIS	-	expression tag	UNP A0A6D0N546
A	-353	HIS	-	expression tag	UNP A0A6D0N546
A	-352	HIS	-	expression tag	UNP A0A6D0N546
A	-351	HIS	-	expression tag	UNP A0A6D0N546
A	-350	HIS	-	expression tag	UNP A0A6D0N546
A	-349	GLU	-	expression tag	UNP A0A6D0N546
A	-348	ASN	-	expression tag	UNP A0A6D0N546
A	-347	LEU	-	expression tag	UNP A0A6D0N546
A	-346	TYR	-	expression tag	UNP A0A6D0N546
A	-345	PHE	-	expression tag	UNP A0A6D0N546
A	-344	GLN	-	expression tag	UNP A0A6D0N546
A	-343	GLY	-	expression tag	UNP A0A6D0N546
A	-171	ALA	GLU	engineered mutation	UNP A0A6D0N546
A	-170	ALA	ASN	engineered mutation	UNP A0A6D0N546
A	-104	ALA	LYS	engineered mutation	UNP A0A6D0N546
A	157	ALA	ILE	engineered mutation	UNP P30550
A	342	GLY	-	expression tag	UNP P30550
A	343	SER	-	expression tag	UNP P30550
A	344	SER	-	expression tag	UNP P30550
A	345	GLY	-	expression tag	UNP P30550
A	346	GLY	-	expression tag	UNP P30550
A	347	GLY	-	expression tag	UNP P30550
A	348	GLY	-	expression tag	UNP P30550
A	349	SER	-	expression tag	UNP P30550
A	350	GLY	-	expression tag	UNP P30550
A	351	GLY	-	expression tag	UNP P30550
A	352	GLY	-	expression tag	UNP P30550
A	353	GLY	-	expression tag	UNP P30550
A	354	SER	-	expression tag	UNP P30550
A	355	SER	-	expression tag	UNP P30550
A	356	GLY	-	expression tag	UNP P30550
A	357	PHE	-	expression tag	UNP P30550
A	358	THR	-	expression tag	UNP P30550
A	359	LEU	-	expression tag	UNP P30550
A	360	GLU	-	expression tag	UNP P30550
A	361	ASP	-	expression tag	UNP P30550
A	362	PHE	-	expression tag	UNP P30550
A	363	VAL	-	expression tag	UNP P30550
A	364	GLY	-	expression tag	UNP P30550
A	365	ASP	-	expression tag	UNP P30550

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Chain	Residue	Modelled	Actual	Comment	Reference
A	366	TRP	-	expression tag	UNP P30550
A	367	GLU	-	expression tag	UNP P30550
A	368	GLN	-	expression tag	UNP P30550
A	369	THR	-	expression tag	UNP P30550
A	370	ALA	-	expression tag	UNP P30550
A	371	ALA	-	expression tag	UNP P30550
A	372	TYR	-	expression tag	UNP P30550
A	373	ASN	-	expression tag	UNP P30550
A	374	LEU	-	expression tag	UNP P30550
A	375	ASP	-	expression tag	UNP P30550
A	376	GLN	-	expression tag	UNP P30550
A	377	VAL	-	expression tag	UNP P30550
A	378	LEU	-	expression tag	UNP P30550
A	379	GLU	-	expression tag	UNP P30550
A	380	GLN	-	expression tag	UNP P30550
A	381	GLY	-	expression tag	UNP P30550
A	382	GLY	-	expression tag	UNP P30550
A	383	VAL	-	expression tag	UNP P30550
A	384	SER	-	expression tag	UNP P30550
A	385	SER	-	expression tag	UNP P30550
A	386	LEU	-	expression tag	UNP P30550
A	387	LEU	-	expression tag	UNP P30550
A	388	GLN	-	expression tag	UNP P30550
A	389	ASN	-	expression tag	UNP P30550
A	390	LEU	-	expression tag	UNP P30550
A	391	ALA	-	expression tag	UNP P30550
A	392	VAL	-	expression tag	UNP P30550
A	393	SER	-	expression tag	UNP P30550
A	394	VAL	-	expression tag	UNP P30550
A	395	THR	-	expression tag	UNP P30550
A	396	PRO	-	expression tag	UNP P30550
A	397	ILE	-	expression tag	UNP P30550
A	398	GLN	-	expression tag	UNP P30550
A	399	ARG	-	expression tag	UNP P30550
A	400	ILE	-	expression tag	UNP P30550
A	401	VAL	-	expression tag	UNP P30550
A	402	ARG	-	expression tag	UNP P30550
A	403	SER	-	expression tag	UNP P30550
A	404	GLY	-	expression tag	UNP P30550
A	405	GLU	-	expression tag	UNP P30550
A	406	ASN	-	expression tag	UNP P30550
A	407	ALA	-	expression tag	UNP P30550

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Chain	Residue	Modelled	Actual	Comment	Reference
A	408	LEU	-	expression tag	UNP P30550
A	409	LYS	-	expression tag	UNP P30550
A	410	ILE	-	expression tag	UNP P30550
A	411	ASP	-	expression tag	UNP P30550
A	412	ILE	-	expression tag	UNP P30550
A	413	HIS	-	expression tag	UNP P30550
A	414	VAL	-	expression tag	UNP P30550
A	415	ILE	-	expression tag	UNP P30550
A	416	ILE	-	expression tag	UNP P30550
A	417	PRO	-	expression tag	UNP P30550
A	418	TYR	-	expression tag	UNP P30550
A	419	GLU	-	expression tag	UNP P30550
A	420	GLY	-	expression tag	UNP P30550
A	421	LEU	-	expression tag	UNP P30550
A	422	SER	-	expression tag	UNP P30550
A	423	ALA	-	expression tag	UNP P30550
A	424	ASP	-	expression tag	UNP P30550
A	425	GLN	-	expression tag	UNP P30550
A	426	MET	-	expression tag	UNP P30550
A	427	ALA	-	expression tag	UNP P30550
A	428	GLN	-	expression tag	UNP P30550
A	429	ILE	-	expression tag	UNP P30550
A	430	GLU	-	expression tag	UNP P30550
A	431	GLU	-	expression tag	UNP P30550
A	432	VAL	-	expression tag	UNP P30550
A	433	PHE	-	expression tag	UNP P30550
A	434	LYS	-	expression tag	UNP P30550
A	435	VAL	-	expression tag	UNP P30550
A	436	VAL	-	expression tag	UNP P30550
A	437	TYR	-	expression tag	UNP P30550
A	438	PRO	-	expression tag	UNP P30550
A	439	VAL	-	expression tag	UNP P30550
A	440	ASP	-	expression tag	UNP P30550
A	441	ASP	-	expression tag	UNP P30550
A	442	HIS	-	expression tag	UNP P30550
A	443	HIS	-	expression tag	UNP P30550
A	444	PHE	-	expression tag	UNP P30550
A	445	LYS	-	expression tag	UNP P30550
A	446	VAL	-	expression tag	UNP P30550
A	447	ILE	-	expression tag	UNP P30550
A	448	LEU	-	expression tag	UNP P30550
A	449	PRO	-	expression tag	UNP P30550

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Chain	Residue	Modelled	Actual	Comment	Reference
A	450	TYR	-	expression tag	UNP P30550
A	451	GLY	-	expression tag	UNP P30550
A	452	THR	-	expression tag	UNP P30550
A	453	LEU	-	expression tag	UNP P30550
A	454	VAL	-	expression tag	UNP P30550
A	455	ILE	-	expression tag	UNP P30550
A	456	ASP	-	expression tag	UNP P30550
A	457	GLY	-	expression tag	UNP P30550
A	458	VAL	-	expression tag	UNP P30550
A	459	THR	-	expression tag	UNP P30550
A	460	PRO	-	expression tag	UNP P30550
A	461	ASN	-	expression tag	UNP P30550
A	462	MET	-	expression tag	UNP P30550
A	463	LEU	-	expression tag	UNP P30550
A	464	ASN	-	expression tag	UNP P30550
A	465	TYR	-	expression tag	UNP P30550
A	466	PHE	-	expression tag	UNP P30550
A	467	GLY	-	expression tag	UNP P30550
A	468	ARG	-	expression tag	UNP P30550
A	469	PRO	-	expression tag	UNP P30550
A	470	TYR	-	expression tag	UNP P30550
A	471	GLU	-	expression tag	UNP P30550
A	472	GLY	-	expression tag	UNP P30550
A	473	ILE	-	expression tag	UNP P30550
A	474	ALA	-	expression tag	UNP P30550
A	475	VAL	-	expression tag	UNP P30550
A	476	PHE	-	expression tag	UNP P30550
A	477	ASP	-	expression tag	UNP P30550
A	478	GLY	-	expression tag	UNP P30550
A	479	LYS	-	expression tag	UNP P30550
A	480	LYS	-	expression tag	UNP P30550
A	481	ILE	-	expression tag	UNP P30550
A	482	THR	-	expression tag	UNP P30550
A	483	VAL	-	expression tag	UNP P30550
A	484	THR	-	expression tag	UNP P30550
A	485	GLY	-	expression tag	UNP P30550
A	486	THR	-	expression tag	UNP P30550
A	487	LEU	-	expression tag	UNP P30550
A	488	TRP	-	expression tag	UNP P30550
A	489	ASN	-	expression tag	UNP P30550
A	490	GLY	-	expression tag	UNP P30550
A	491	ASN	-	expression tag	UNP P30550

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Chain	Residue	Modelled	Actual	Comment	Reference
A	492	LYS	-	expression tag	UNP P30550
A	493	ILE	-	expression tag	UNP P30550
A	494	ILE	-	expression tag	UNP P30550
A	495	ASP	-	expression tag	UNP P30550
A	496	GLU	-	expression tag	UNP P30550
A	497	ARG	-	expression tag	UNP P30550
A	498	LEU	-	expression tag	UNP P30550
A	499	ILE	-	expression tag	UNP P30550
A	500	THR	-	expression tag	UNP P30550
A	501	PRO	-	expression tag	UNP P30550
A	502	ASP	-	expression tag	UNP P30550
A	503	GLY	-	expression tag	UNP P30550
A	504	SER	-	expression tag	UNP P30550
A	505	MET	-	expression tag	UNP P30550
A	506	LEU	-	expression tag	UNP P30550
A	507	PHE	-	expression tag	UNP P30550
A	508	ARG	-	expression tag	UNP P30550
A	509	VAL	-	expression tag	UNP P30550
A	510	THR	-	expression tag	UNP P30550
A	511	ILE	-	expression tag	UNP P30550
A	512	ASN	-	expression tag	UNP P30550
A	513	SER	-	expression tag	UNP P30550

- Molecule 2 is a protein called Guanine nucleotide-binding protein G(q) subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	283	Total	C	N	O	S	0	0
			2330	1480	396	443	11		

There are 31 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	7	MET	-	initiating methionine	UNP P50148
B	8	GLY	-	expression tag	UNP P50148
B	9	CYS	-	expression tag	UNP P50148
B	10	THR	-	expression tag	UNP P50148
B	11	LEU	-	expression tag	UNP P50148
B	12	SER	-	expression tag	UNP P50148
B	13	ALA	-	expression tag	UNP P50148
B	14	GLU	-	expression tag	UNP P50148
B	15	ASP	-	expression tag	UNP P50148
B	16	LYS	-	expression tag	UNP P50148

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Chain	Residue	Modelled	Actual	Comment	Reference
B	17	ALA	-	expression tag	UNP P50148
B	18	ALA	-	expression tag	UNP P50148
B	19	VAL	-	expression tag	UNP P50148
B	20	GLU	-	expression tag	UNP P50148
B	21	ARG	-	expression tag	UNP P50148
B	22	SER	-	expression tag	UNP P50148
B	23	LYS	-	expression tag	UNP P50148
B	24	MET	-	expression tag	UNP P50148
B	25	ILE	-	expression tag	UNP P50148
B	26	ASP	-	expression tag	UNP P50148
B	27	ARG	-	expression tag	UNP P50148
B	28	ASN	-	expression tag	UNP P50148
B	29	LEU	-	expression tag	UNP P50148
B	30	ARG	-	expression tag	UNP P50148
B	31	GLU	-	expression tag	UNP P50148
B	32	ASP	-	expression tag	UNP P50148
B	33	GLY	-	expression tag	UNP P50148
B	34	GLU	-	expression tag	UNP P50148
B	35	LYS	-	expression tag	UNP P50148
B	183	GLN	ARG	engineered mutation	UNP P50148
B	209	LEU	GLN	engineered mutation	UNP P50148

- Molecule 3 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	315	Total	C	N	O	S	0	0
			2409	1491	428	470	20		

There are 41 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-13	MET	-	initiating methionine	UNP P62873
C	-12	HIS	-	expression tag	UNP P62873
C	-11	HIS	-	expression tag	UNP P62873
C	-10	HIS	-	expression tag	UNP P62873
C	-9	HIS	-	expression tag	UNP P62873
C	-8	HIS	-	expression tag	UNP P62873
C	-7	HIS	-	expression tag	UNP P62873
C	-6	HIS	-	expression tag	UNP P62873
C	-5	HIS	-	expression tag	UNP P62873
C	-4	HIS	-	expression tag	UNP P62873

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	HIS	-	expression tag	UNP P62873
C	-2	GLY	-	expression tag	UNP P62873
C	-1	SER	-	expression tag	UNP P62873
C	0	SER	-	expression tag	UNP P62873
C	1	GLY	-	expression tag	UNP P62873
C	341	GLY	-	expression tag	UNP P62873
C	342	SER	-	expression tag	UNP P62873
C	343	SER	-	expression tag	UNP P62873
C	344	GLY	-	expression tag	UNP P62873
C	345	GLY	-	expression tag	UNP P62873
C	346	GLY	-	expression tag	UNP P62873
C	347	GLY	-	expression tag	UNP P62873
C	348	SER	-	expression tag	UNP P62873
C	349	GLY	-	expression tag	UNP P62873
C	350	GLY	-	expression tag	UNP P62873
C	351	GLY	-	expression tag	UNP P62873
C	352	GLY	-	expression tag	UNP P62873
C	353	SER	-	expression tag	UNP P62873
C	354	SER	-	expression tag	UNP P62873
C	355	GLY	-	expression tag	UNP P62873
C	356	VAL	-	expression tag	UNP P62873
C	357	SER	-	expression tag	UNP P62873
C	358	GLY	-	expression tag	UNP P62873
C	359	TRP	-	expression tag	UNP P62873
C	360	ARG	-	expression tag	UNP P62873
C	361	LEU	-	expression tag	UNP P62873
C	362	PHE	-	expression tag	UNP P62873
C	363	LYS	-	expression tag	UNP P62873
C	364	LYS	-	expression tag	UNP P62873
C	365	ILE	-	expression tag	UNP P62873
C	366	SER	-	expression tag	UNP P62873

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	47	Total	C	N	O	S	0	0
			365	228	62	72	3		

There are 11 discrepancies between the modelled and reference sequences:

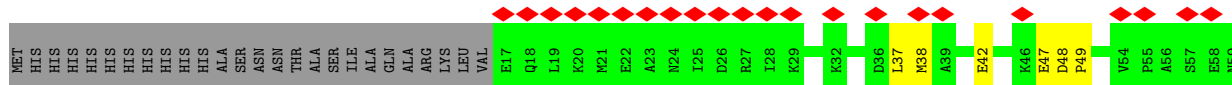
Chain	Residue	Modelled	Actual	Comment	Reference
D	-9	MET	-	initiating methionine	UNP P59768
D	-8	HIS	-	expression tag	UNP P59768
D	-7	HIS	-	expression tag	UNP P59768
D	-6	HIS	-	expression tag	UNP P59768
D	-5	HIS	-	expression tag	UNP P59768
D	-4	HIS	-	expression tag	UNP P59768
D	-3	HIS	-	expression tag	UNP P59768
D	-2	HIS	-	expression tag	UNP P59768
D	-1	HIS	-	expression tag	UNP P59768
D	0	HIS	-	expression tag	UNP P59768
D	1	HIS	-	expression tag	UNP P59768

- Molecule 5 is a protein called ScFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	H	230	Total	C	N	O	S	0	0
			1771	1123	293	345	10		

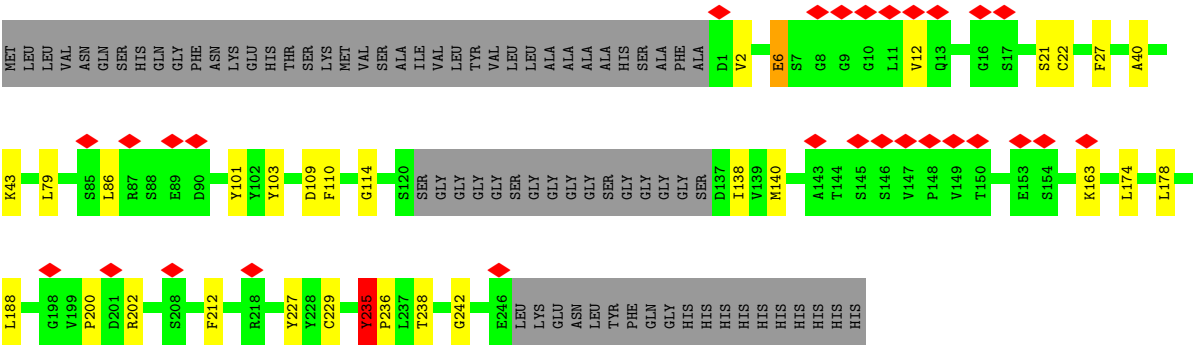
- Molecule 6 is a protein called Bombesin.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	9	Total	C	N	O	0	0
			81	57	14	10		

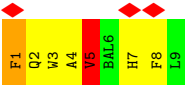




● Molecule 5: ScFv16



● Molecule 6: Bombesin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	1380329	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	64	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 BASE (4k x 4k)	Depositor
Maximum map value	0.181	Depositor
Minimum map value	-0.137	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size ($\text{\AA}$)	243.36002, 243.36002, 243.36002	wwPDB
Map dimensions	240, 240, 240	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.014, 1.014, 1.014	Depositor

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: BAL, DPN, NLN

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	0.81	0/2342	1.04	2/3196 (0.1%)
2	B	0.64	0/2371	0.87	0/3190
3	C	0.68	0/2456	0.92	2/3335 (0.1%)
4	D	0.51	0/371	0.66	0/501
5	H	0.69	0/1815	0.87	1/2461 (0.0%)
6	E	1.77	2/58 (3.4%)	1.52	0/77
All	All	0.72	2/9413 (0.0%)	0.93	5/12760 (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
6	E	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	3	TRP	CG-CD2	-5.54	1.33	1.43
6	E	8	PHE	CB-CG	-5.07	1.39	1.50

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	247	ASP	N-CA-C	-6.03	102.15	110.35
1	A	176	ALA	N-CA-C	-5.61	106.80	113.97
5	H	114	GLY	CA-C-O	-5.17	117.85	121.88
1	A	205	LEU	N-CA-C	-5.15	107.06	113.55
3	C	48	ARG	N-CA-C	-5.15	106.84	113.23

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
6	E	5	VAL	Peptide

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	2280	0	2226	43	0
2	B	2330	0	2313	33	0
3	C	2409	0	2312	52	0
4	D	365	0	362	11	0
5	H	1771	0	1703	21	0
6	E	81	0	74	4	0
All	All	9236	0	8990	135	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 7.

The worst 5 of 135 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:242:TYR:OH	1:A:260:LYS:HE2	1.75	0.86
1:A:40:LEU:O	1:A:44:PRO:HD2	1.85	0.75
1:A:242:TYR:CZ	1:A:260:LYS:HE2	2.23	0.72
3:C:130:GLU:HB3	5:H:27:PHE:HA	1.72	0.70
1:A:242:TYR:CE1	1:A:260:LYS:CE	2.78	0.67

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	299/897 (33%)	291 (97%)	8 (3%)	0	100	100
2	B	277/353 (78%)	270 (98%)	7 (2%)	0	100	100
3	C	313/380 (82%)	304 (97%)	9 (3%)	0	100	100
4	D	45/81 (56%)	44 (98%)	1 (2%)	0	100	100
5	H	226/303 (75%)	220 (97%)	5 (2%)	1 (0%)	30	65
6	E	6/9 (67%)	3 (50%)	1 (17%)	2 (33%)	0	0
All	All	1166/2023 (58%)	1132 (97%)	31 (3%)	3 (0%)	37	70

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
6	E	4	ALA
6	E	7	HIS
5	H	235	TYR

5.3.2 Protein sidechains ⓘ

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	230/753 (30%)	225 (98%)	5 (2%)	45	74
2	B	259/319 (81%)	252 (97%)	7 (3%)	39	71
3	C	261/310 (84%)	257 (98%)	4 (2%)	57	80
4	D	39/68 (57%)	39 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	H	195/247 (79%)	193 (99%)	2 (1%)	68	84
6	E	5/5 (100%)	4 (80%)	1 (20%)	1	7
All	All	989/1702 (58%)	970 (98%)	19 (2%)	49	76

5 of 19 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	294	CYS
5	H	235	TYR
6	E	5	VAL
5	H	6	GLU
2	B	288	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	C	183	HIS
3	C	220	GLN
5	H	39	GLN
1	A	236	ASN
1	A	201	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NLN	E	9	6	8,8,8	0.36	0	8,9,9	0.67	0
6	BAL	E	6	6	3,4,5	0.41	0	3,3,5	0.70	0
6	DPN	E	1	6	10,11,12	1.63	1 (10%)	8,13,15	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NLN	E	9	6	-	0/8/8/8	-
6	BAL	E	6	6	-	1/1/2/3	-
6	DPN	E	1	6	-	3/5/6/8	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	1	DPN	CB-CG	-4.99	1.39	1.51

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	E	1	DPN	O-C-CA-CB
6	E	1	DPN	CA-CB-CG-CD1
6	E	1	DPN	CA-CB-CG-CD2
6	E	6	BAL	C-CA-CB-N

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	E	1	DPN	1	0

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.

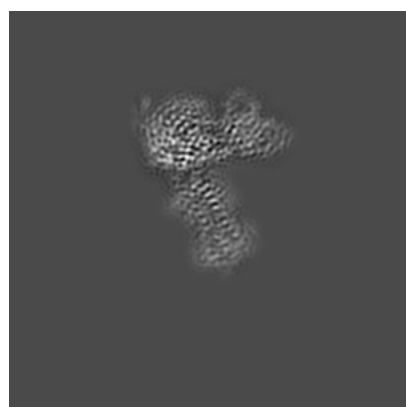
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32298. These allow visual inspection of the internal detail of the map and identification of artifacts.

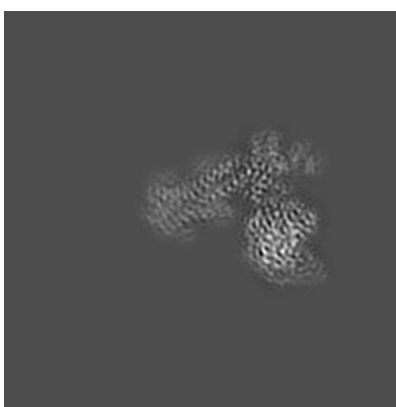
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

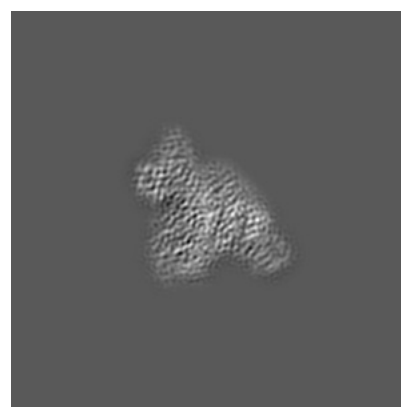
6.1.1 Primary map



X



Y

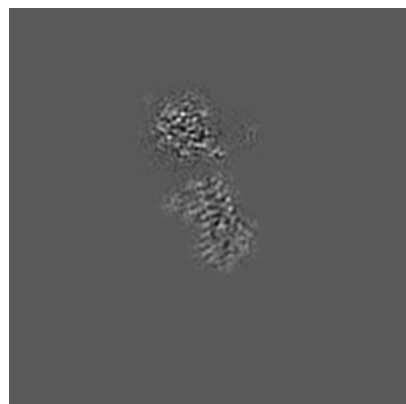


Z

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

6.2 Central slices [i](#)

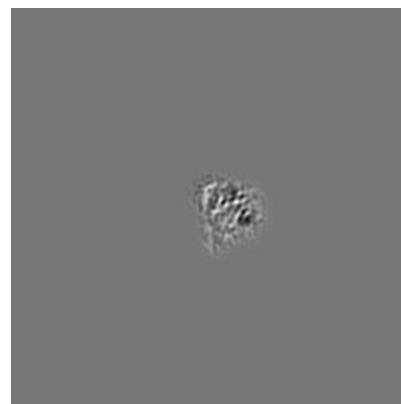
6.2.1 Primary map



X Index: 120



Y Index: 120

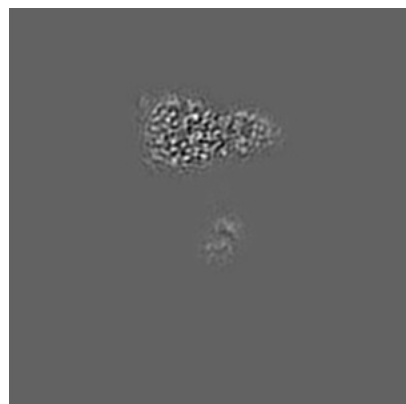


Z Index: 120

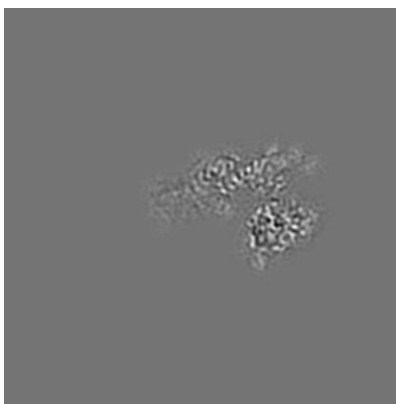
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

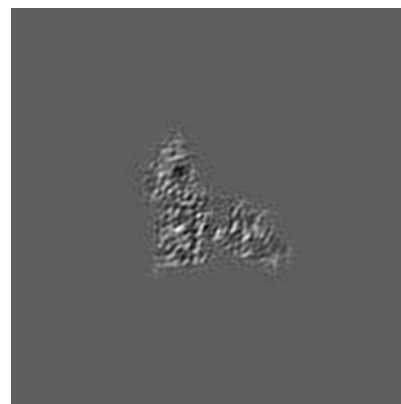
6.3.1 Primary map



X Index: 107



Y Index: 113

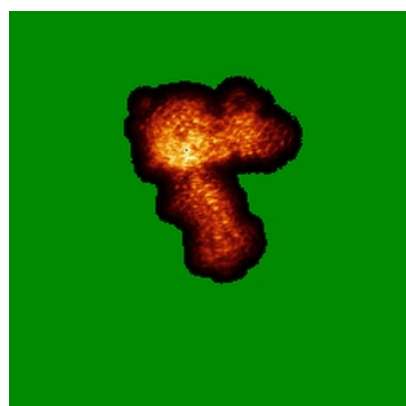


Z Index: 156

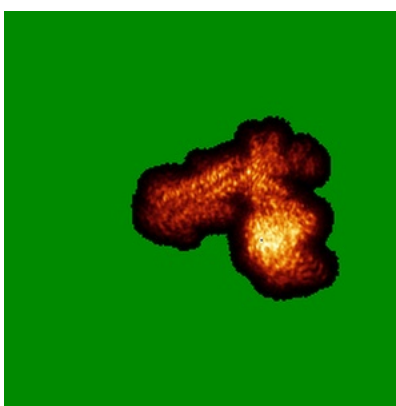
The images above show the largest variance slices of the map in three orthogonal directions.

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

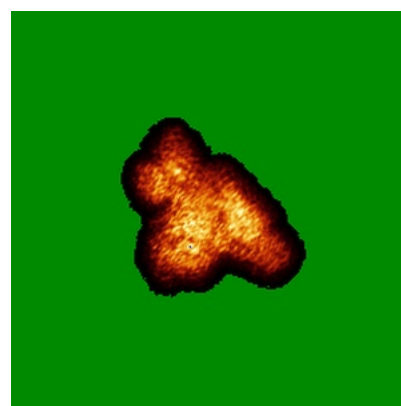
6.4.1 Primary map



X



Y

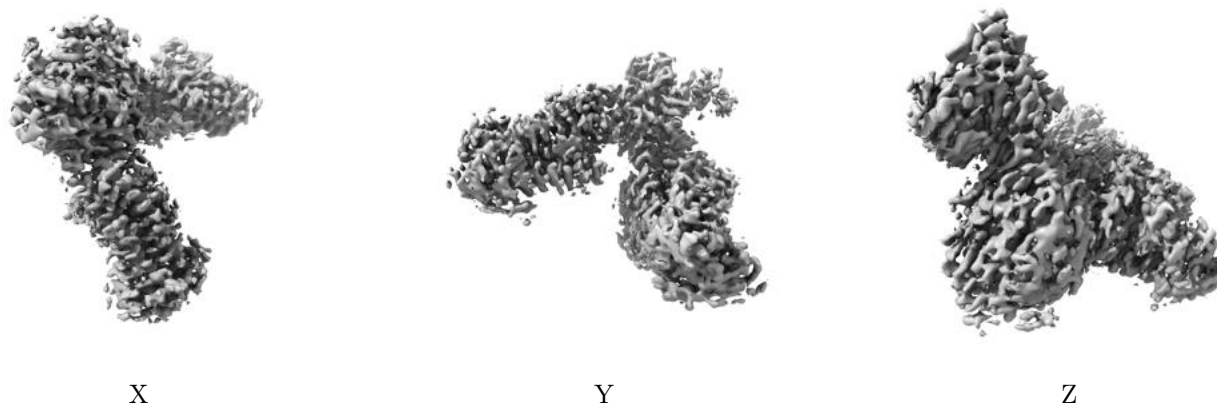


Z

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

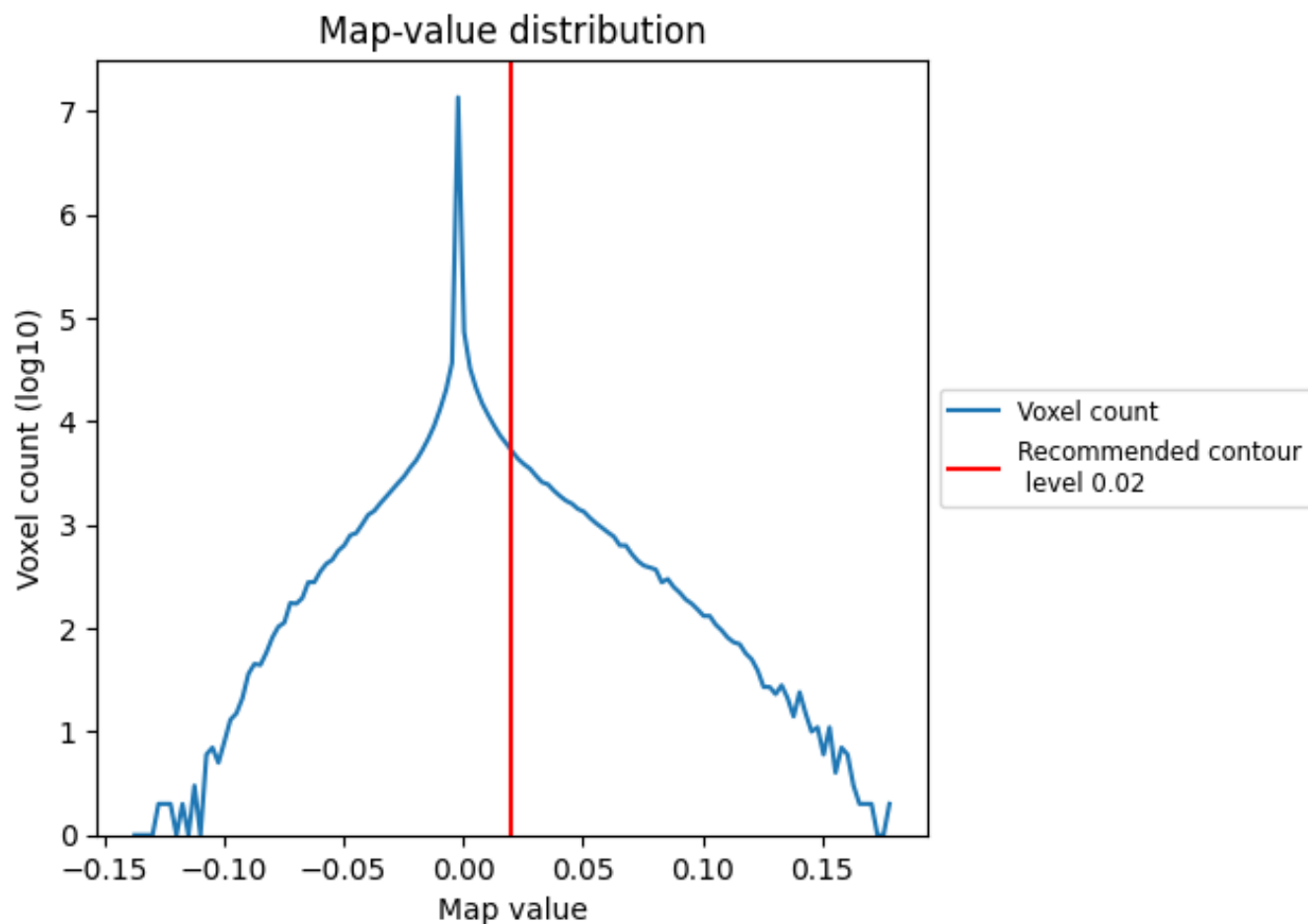
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

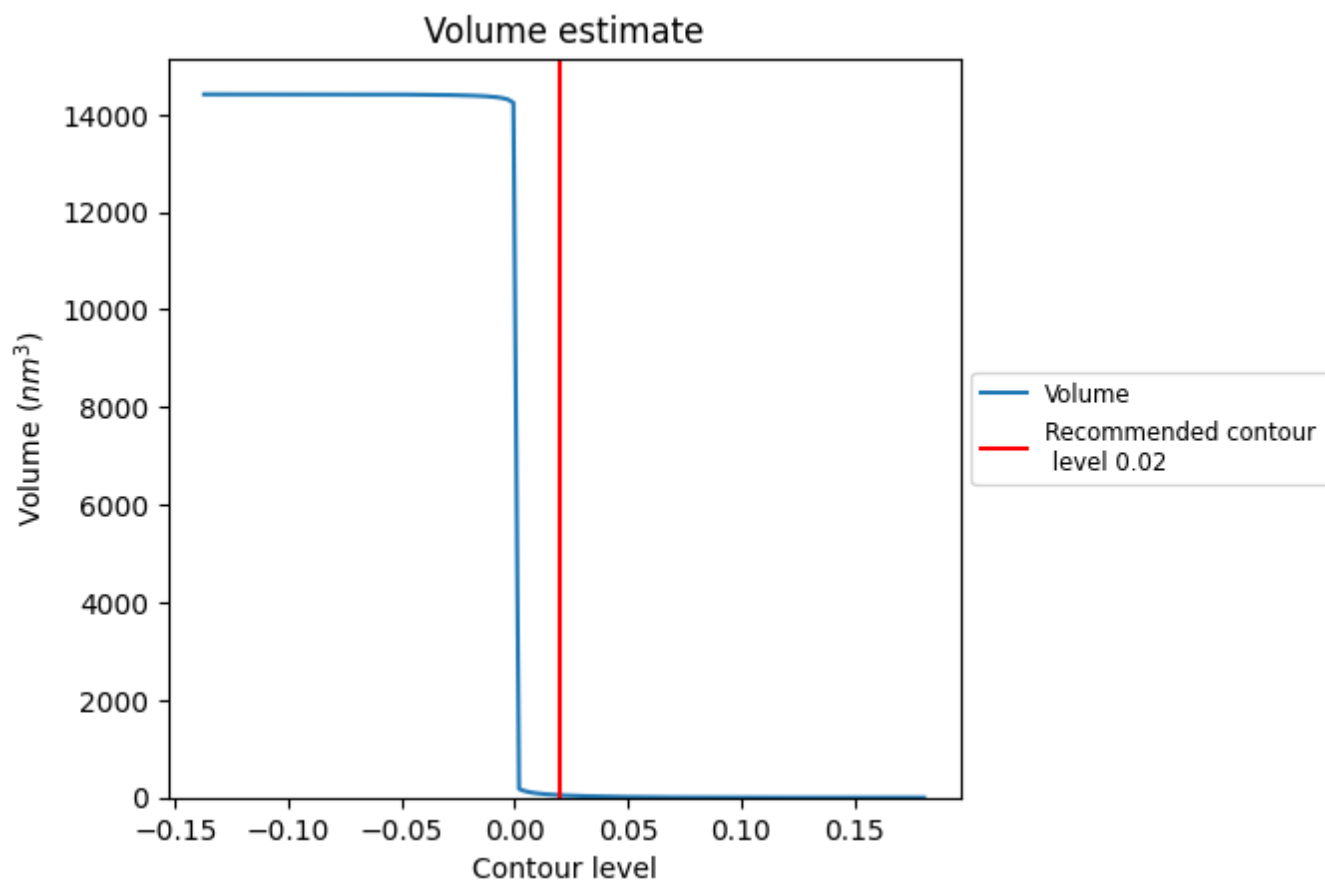
This section contains the results of statistical analysis of the map.

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.

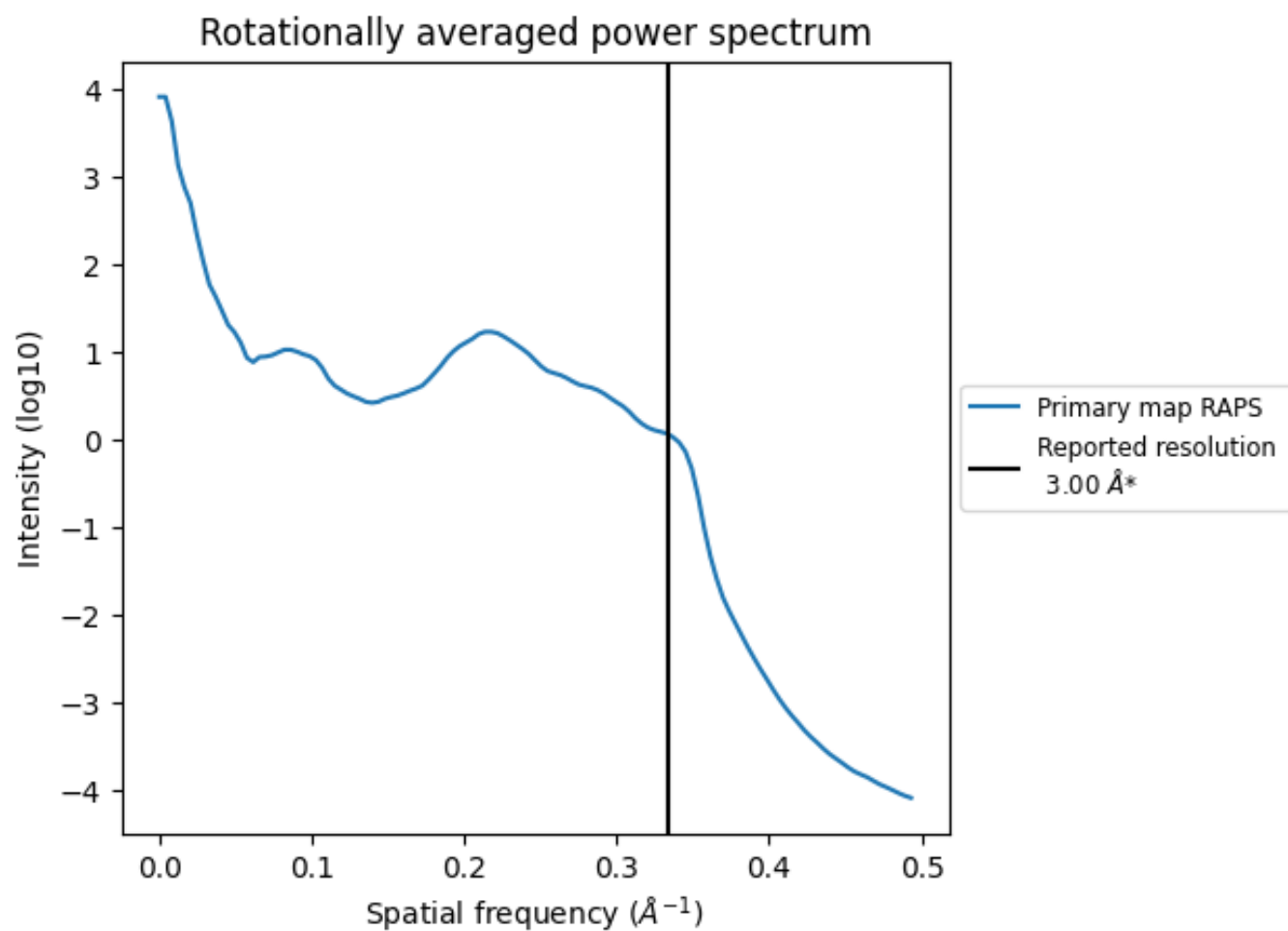
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 49 nm³; this corresponds to an approximate mass of 44 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⁻¹

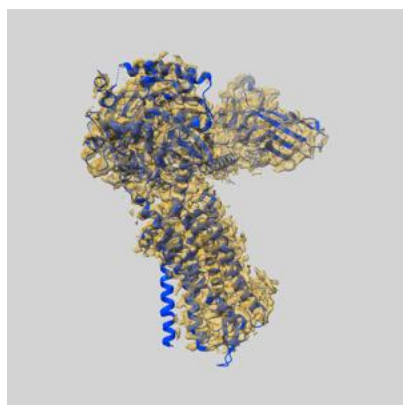
8 Fourier-Shell correlation

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

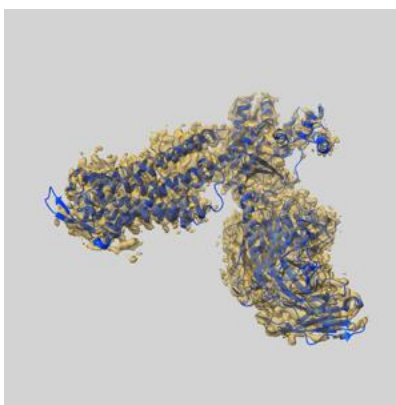
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32298 and PDB model 7W40. Per-residue inclusion information can be found in [section 3](#) on [page 13](#).

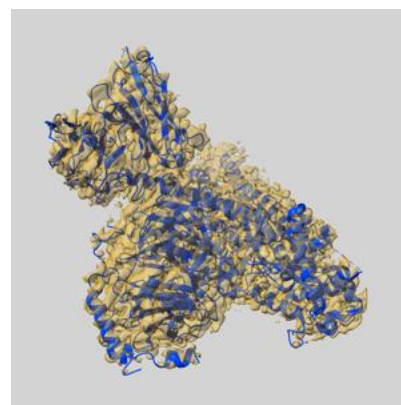
9.1 Map-model overlay [i](#)



X



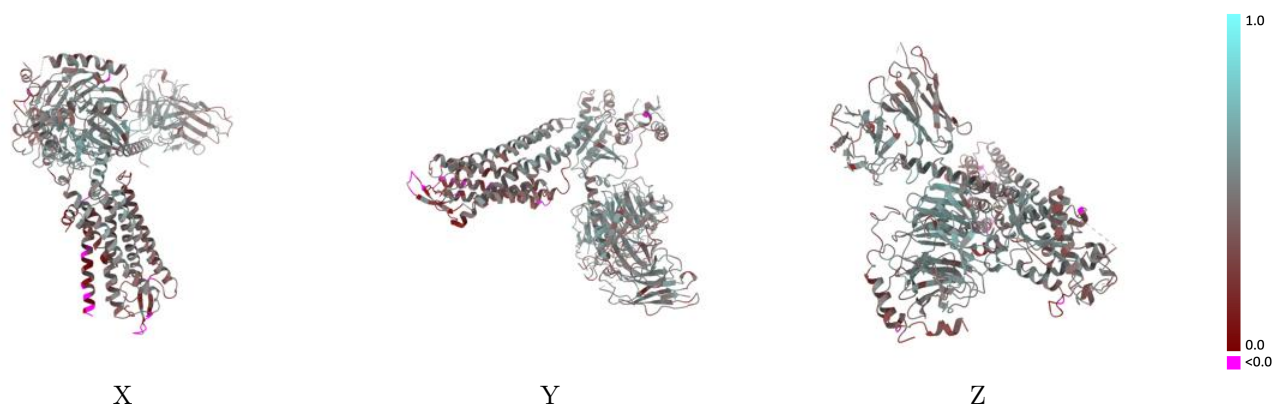
Y



Z

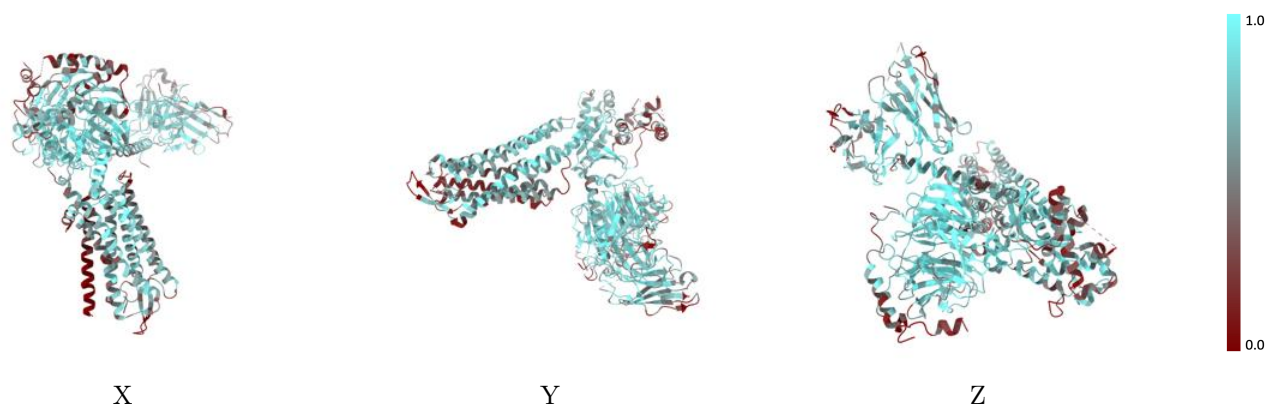
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



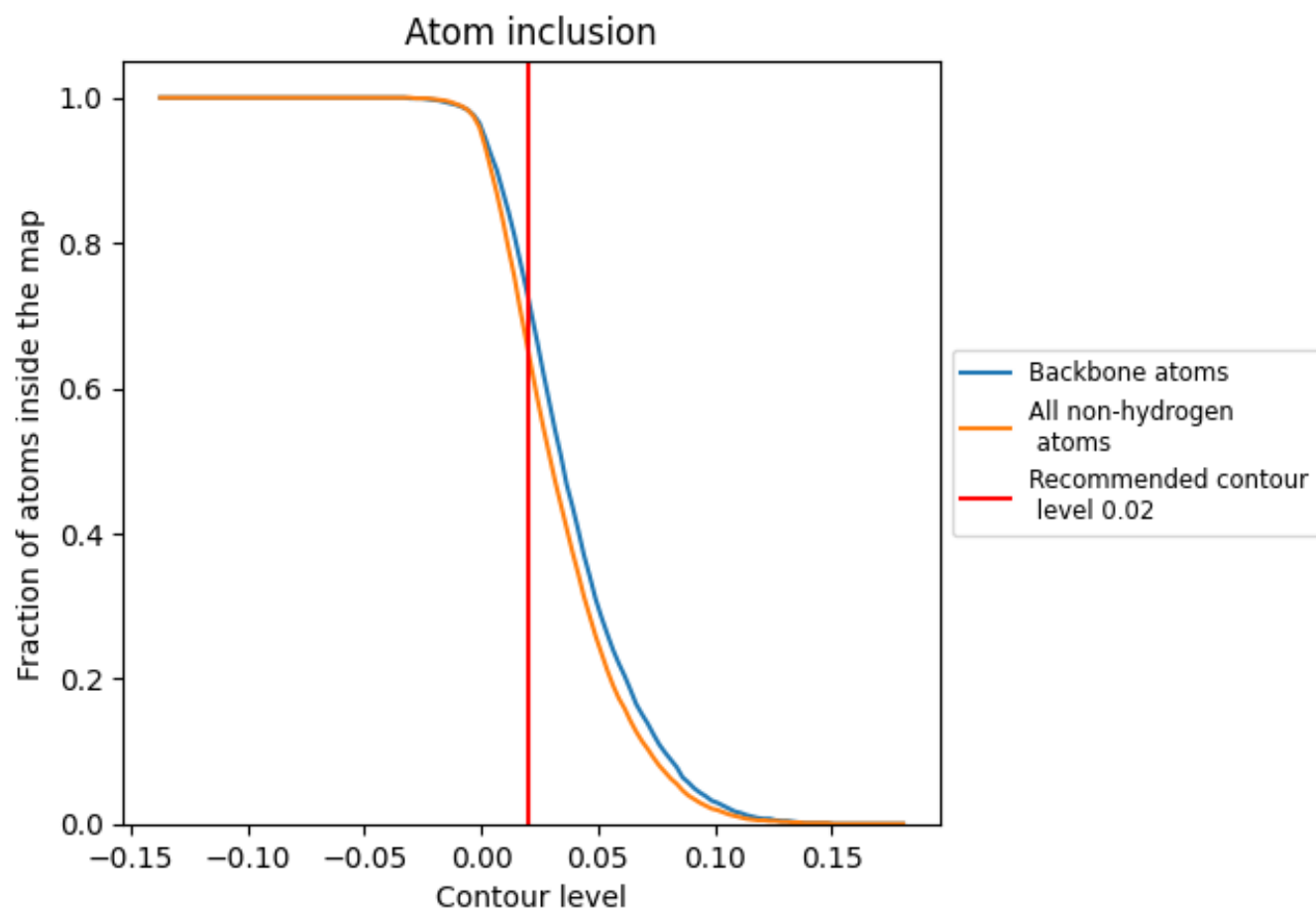
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 66% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6550	0.4370
A	0.5550	0.3610
B	0.6350	0.4560
C	0.7920	0.4940
D	0.4110	0.3570
E	0.4940	0.2710
H	0.6830	0.4550

