Full wwPDB EM Validation Report ⓘ

Apr 25, 2026 – 10:59 PM EDT

PDB ID	:	9OXB / pdb_00009oxb
EMDB ID	:	EMD-70965
Title	:	CryoEM structure of Ggust-coupled TAS2R43 with aristolochic acid I
Authors	:	Kim, Y.; Gumpper, R.H.; Roth, B.L.
Deposited on	:	2025-06-03
Resolution	:	3.00 Å(reported)

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

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

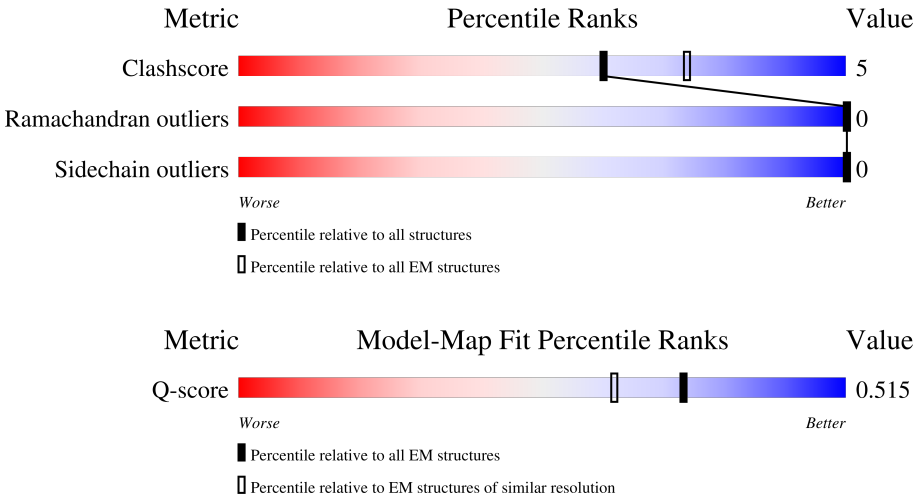
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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

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 <=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	354	8% 56% 8% 37%
2	B	402	76% 8% 16%
3	C	71	7% 65% 6% 30%
4	D	267	76% 11% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	R	645	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 8532 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(t) subunit alpha-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	224	1711	1093	287	318	13	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	4	THR	GLY	conflict	UNP A8MTJ3
A	5	VAL	ILE	conflict	UNP A8MTJ3
A	7	ALA	SER	conflict	UNP A8MTJ3
A	9	ASP	SER	conflict	UNP A8MTJ3
A	11	ALA	GLU	conflict	UNP A8MTJ3
A	12	ALA	SER	conflict	UNP A8MTJ3
A	14	GLU	LYS	conflict	UNP A8MTJ3
A	18	MET	GLU	conflict	UNP A8MTJ3
A	19	ILE	LEU	conflict	UNP A8MTJ3
A	20	ASP	GLU	conflict	UNP A8MTJ3
A	22	ASN	LYS	conflict	UNP A8MTJ3
A	24	ARG	GLN	conflict	UNP A8MTJ3
A	47	ALA	SER	conflict	UNP A8MTJ3
A	53	GLN	MET	conflict	UNP A8MTJ3
A	54	MET	LYS	conflict	UNP A8MTJ3
A	203	ALA	GLY	conflict	UNP A8MTJ3
A	245	ALA	GLU	conflict	UNP A8MTJ3
A	248	LYS	HIS	conflict	UNP A8MTJ3
A	251	ASP	ASN	conflict	UNP A8MTJ3
A	261	ASP	THR	conflict	UNP A8MTJ3
A	326	SER	ALA	conflict	UNP A8MTJ3

- 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	338	Total	C	N	O	S	0	0
			2458	1530	429	478	21		

There are 63 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-17	MET	-	expression tag	UNP P62873
B	-16	HIS	-	expression tag	UNP P62873
B	-15	HIS	-	expression tag	UNP P62873
B	-14	HIS	-	expression tag	UNP P62873
B	-13	HIS	-	expression tag	UNP P62873
B	-12	HIS	-	expression tag	UNP P62873
B	-11	HIS	-	expression tag	UNP P62873
B	-10	LEU	-	expression tag	UNP P62873
B	-9	GLU	-	expression tag	UNP P62873
B	-8	VAL	-	expression tag	UNP P62873
B	-7	LEU	-	expression tag	UNP P62873
B	-6	PHE	-	expression tag	UNP P62873
B	-5	GLN	-	expression tag	UNP P62873
B	-4	GLY	-	expression tag	UNP P62873
B	-3	PRO	-	expression tag	UNP P62873
B	-2	GLY	-	expression tag	UNP P62873
B	-1	SER	-	expression tag	UNP P62873
B	0	SER	-	expression tag	UNP P62873
B	1	GLY	-	expression tag	UNP P62873
B	341	GLY	-	expression tag	UNP P62873
B	342	GLY	-	expression tag	UNP P62873
B	343	SER	-	expression tag	UNP P62873
B	344	GLY	-	expression tag	UNP P62873
B	345	GLY	-	expression tag	UNP P62873
B	346	GLY	-	expression tag	UNP P62873
B	347	GLY	-	expression tag	UNP P62873
B	348	SER	-	expression tag	UNP P62873
B	349	GLY	-	expression tag	UNP P62873
B	350	GLY	-	expression tag	UNP P62873
B	351	SER	-	expression tag	UNP P62873
B	352	SER	-	expression tag	UNP P62873
B	353	SER	-	expression tag	UNP P62873
B	354	GLY	-	expression tag	UNP P62873
B	355	GLY	-	expression tag	UNP P62873
B	356	GLY	-	expression tag	UNP P62873
B	357	GLY	-	expression tag	UNP P62873
B	358	SER	-	expression tag	UNP P62873

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	359	GLY	-	expression tag	UNP P62873
B	360	GLY	-	expression tag	UNP P62873
B	361	GLY	-	expression tag	UNP P62873
B	362	GLY	-	expression tag	UNP P62873
B	363	SER	-	expression tag	UNP P62873
B	364	GLY	-	expression tag	UNP P62873
B	365	GLY	-	expression tag	UNP P62873
B	366	SER	-	expression tag	UNP P62873
B	367	SER	-	expression tag	UNP P62873
B	368	SER	-	expression tag	UNP P62873
B	369	GLY	-	expression tag	UNP P62873
B	370	GLY	-	expression tag	UNP P62873
B	371	VAL	-	expression tag	UNP P62873
B	372	SER	-	expression tag	UNP P62873
B	373	GLY	-	expression tag	UNP P62873
B	374	TRP	-	expression tag	UNP P62873
B	375	ARG	-	expression tag	UNP P62873
B	376	LEU	-	expression tag	UNP P62873
B	377	PHE	-	expression tag	UNP P62873
B	378	LYS	-	expression tag	UNP P62873
B	379	LYS	-	expression tag	UNP P62873
B	380	ILE	-	expression tag	UNP P62873
B	381	SER	-	expression tag	UNP P62873
B	382	GLY	-	expression tag	UNP P62873
B	383	GLY	-	expression tag	UNP P62873
B	384	SER	-	expression tag	UNP P62873

- 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	C	50	Total	C	N	O	S	0	0
			328	209	57	59	3		

- Molecule 4 is a protein called scFv16.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	232	Total	C	N	O	S	0	0
			1761	1119	291	341	10		

- Molecule 5 is a protein called Taste receptor type 2 member 43.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	R	284	Total	C	N	O	S	0	0
			2244	1511	360	359	14		

There are 336 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-150	ASP	-	expression tag	UNP P59537
R	-149	TYR	-	expression tag	UNP P59537
R	-148	LYS	-	expression tag	UNP P59537
R	-147	ASP	-	expression tag	UNP P59537
R	-146	ASP	-	expression tag	UNP P59537
R	-145	ASP	-	expression tag	UNP P59537
R	-144	ASP	-	expression tag	UNP P59537
R	-143	ALA	-	expression tag	UNP P59537
R	-142	LYS	-	expression tag	UNP P59537
R	-141	LEU	-	expression tag	UNP P59537
R	-140	GLN	-	expression tag	UNP P59537
R	-139	THR	-	expression tag	UNP P59537
R	-138	MET	-	expression tag	UNP P59537
R	-137	HIS	-	expression tag	UNP P59537
R	-136	HIS	-	expression tag	UNP P59537
R	-135	HIS	-	expression tag	UNP P59537
R	-134	HIS	-	expression tag	UNP P59537
R	-133	HIS	-	expression tag	UNP P59537
R	-132	HIS	-	expression tag	UNP P59537
R	-131	HIS	-	expression tag	UNP P59537
R	-130	HIS	-	expression tag	UNP P59537
R	-129	HIS	-	expression tag	UNP P59537
R	-128	HIS	-	expression tag	UNP P59537
R	-127	GLU	-	expression tag	UNP P59537
R	-126	ASN	-	expression tag	UNP P59537
R	-125	LEU	-	expression tag	UNP P59537
R	-124	TYR	-	expression tag	UNP P59537
R	-123	PHE	-	expression tag	UNP P59537
R	-122	GLN	-	expression tag	UNP P59537
R	-121	GLY	-	expression tag	UNP P59537
R	-120	GLY	-	expression tag	UNP P59537
R	-119	THR	-	expression tag	UNP P59537
R	-118	THR	-	expression tag	UNP P59537
R	-117	MET	-	expression tag	UNP P59537
R	-116	ALA	-	expression tag	UNP P59537
R	-115	ASP	-	expression tag	UNP P59537
R	-114	LEU	-	expression tag	UNP P59537

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	-113	GLU	-	expression tag	UNP P59537
R	-112	ASP	-	expression tag	UNP P59537
R	-111	ASN	-	expression tag	UNP P59537
R	-110	TRP	-	expression tag	UNP P59537
R	-109	GLU	-	expression tag	UNP P59537
R	-108	THR	-	expression tag	UNP P59537
R	-107	LEU	-	expression tag	UNP P59537
R	-106	ASN	-	expression tag	UNP P59537
R	-105	ASP	-	expression tag	UNP P59537
R	-104	ASN	-	expression tag	UNP P59537
R	-103	LEU	-	expression tag	UNP P59537
R	-102	LYS	-	expression tag	UNP P59537
R	-101	VAL	-	expression tag	UNP P59537
R	-100	ILE	-	expression tag	UNP P59537
R	-99	GLU	-	expression tag	UNP P59537
R	-98	LYS	-	expression tag	UNP P59537
R	-97	ALA	-	expression tag	UNP P59537
R	-96	ASP	-	expression tag	UNP P59537
R	-95	ASN	-	expression tag	UNP P59537
R	-94	ALA	-	expression tag	UNP P59537
R	-93	ALA	-	expression tag	UNP P59537
R	-92	GLN	-	expression tag	UNP P59537
R	-91	VAL	-	expression tag	UNP P59537
R	-90	LYS	-	expression tag	UNP P59537
R	-89	ASP	-	expression tag	UNP P59537
R	-88	ALA	-	expression tag	UNP P59537
R	-87	LEU	-	expression tag	UNP P59537
R	-86	THR	-	expression tag	UNP P59537
R	-85	LYS	-	expression tag	UNP P59537
R	-84	MET	-	expression tag	UNP P59537
R	-83	ARG	-	expression tag	UNP P59537
R	-82	ALA	-	expression tag	UNP P59537
R	-81	ALA	-	expression tag	UNP P59537
R	-80	ALA	-	expression tag	UNP P59537
R	-79	LEU	-	expression tag	UNP P59537
R	-78	ASP	-	expression tag	UNP P59537
R	-77	ALA	-	expression tag	UNP P59537
R	-76	GLN	-	expression tag	UNP P59537
R	-75	LYS	-	expression tag	UNP P59537
R	-74	ALA	-	expression tag	UNP P59537
R	-73	THR	-	expression tag	UNP P59537
R	-72	PRO	-	expression tag	UNP P59537

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	-71	PRO	-	expression tag	UNP P59537
R	-70	LYS	-	expression tag	UNP P59537
R	-69	LEU	-	expression tag	UNP P59537
R	-68	GLU	-	expression tag	UNP P59537
R	-67	ASP	-	expression tag	UNP P59537
R	-66	LYS	-	expression tag	UNP P59537
R	-65	SER	-	expression tag	UNP P59537
R	-64	PRO	-	expression tag	UNP P59537
R	-63	ASP	-	expression tag	UNP P59537
R	-62	SER	-	expression tag	UNP P59537
R	-61	PRO	-	expression tag	UNP P59537
R	-60	GLU	-	expression tag	UNP P59537
R	-59	MET	-	expression tag	UNP P59537
R	-58	LYS	-	expression tag	UNP P59537
R	-57	ASP	-	expression tag	UNP P59537
R	-56	PHE	-	expression tag	UNP P59537
R	-55	ARG	-	expression tag	UNP P59537
R	-54	HIS	-	expression tag	UNP P59537
R	-53	GLY	-	expression tag	UNP P59537
R	-52	PHE	-	expression tag	UNP P59537
R	-51	ASP	-	expression tag	UNP P59537
R	-50	ILE	-	expression tag	UNP P59537
R	-49	LEU	-	expression tag	UNP P59537
R	-48	VAL	-	expression tag	UNP P59537
R	-47	GLY	-	expression tag	UNP P59537
R	-46	GLN	-	expression tag	UNP P59537
R	-45	ILE	-	expression tag	UNP P59537
R	-44	ASP	-	expression tag	UNP P59537
R	-43	ASP	-	expression tag	UNP P59537
R	-42	ALA	-	expression tag	UNP P59537
R	-41	LEU	-	expression tag	UNP P59537
R	-40	LYS	-	expression tag	UNP P59537
R	-39	LEU	-	expression tag	UNP P59537
R	-38	ALA	-	expression tag	UNP P59537
R	-37	ASN	-	expression tag	UNP P59537
R	-36	GLU	-	expression tag	UNP P59537
R	-35	GLY	-	expression tag	UNP P59537
R	-34	LYS	-	expression tag	UNP P59537
R	-33	VAL	-	expression tag	UNP P59537
R	-32	LYS	-	expression tag	UNP P59537
R	-31	GLU	-	expression tag	UNP P59537
R	-30	ALA	-	expression tag	UNP P59537

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	-29	GLN	-	expression tag	UNP P59537
R	-28	ALA	-	expression tag	UNP P59537
R	-27	ALA	-	expression tag	UNP P59537
R	-26	ALA	-	expression tag	UNP P59537
R	-25	GLU	-	expression tag	UNP P59537
R	-24	GLN	-	expression tag	UNP P59537
R	-23	LEU	-	expression tag	UNP P59537
R	-22	LYS	-	expression tag	UNP P59537
R	-21	THR	-	expression tag	UNP P59537
R	-20	THR	-	expression tag	UNP P59537
R	-19	ARG	-	expression tag	UNP P59537
R	-18	ASN	-	expression tag	UNP P59537
R	-17	ALA	-	expression tag	UNP P59537
R	-16	TYR	-	expression tag	UNP P59537
R	-15	ILE	-	expression tag	UNP P59537
R	-14	GLN	-	expression tag	UNP P59537
R	-13	LYS	-	expression tag	UNP P59537
R	-12	TYR	-	expression tag	UNP P59537
R	-11	LEU	-	expression tag	UNP P59537
R	-10	GLY	-	expression tag	UNP P59537
R	-9	SER	-	expression tag	UNP P59537
R	-8	THR	-	expression tag	UNP P59537
R	-7	LEU	-	expression tag	UNP P59537
R	-6	GLU	-	expression tag	UNP P59537
R	-5	VAL	-	expression tag	UNP P59537
R	-4	LEU	-	expression tag	UNP P59537
R	-3	PHE	-	expression tag	UNP P59537
R	-2	GLN	-	expression tag	UNP P59537
R	-1	GLY	-	expression tag	UNP P59537
R	0	PRO	-	expression tag	UNP P59537
R	310	GLY	-	expression tag	UNP P59537
R	311	SER	-	expression tag	UNP P59537
R	312	ALA	-	expression tag	UNP P59537
R	313	GLY	-	expression tag	UNP P59537
R	314	SER	-	expression tag	UNP P59537
R	315	ALA	-	expression tag	UNP P59537
R	316	GLY	-	expression tag	UNP P59537
R	317	SER	-	expression tag	UNP P59537
R	318	GLY	-	expression tag	UNP P59537
R	319	GLY	-	expression tag	UNP P59537
R	320	SER	-	expression tag	UNP P59537
R	321	GLY	-	expression tag	UNP P59537

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	322	GLY	-	expression tag	UNP P59537
R	323	GLY	-	expression tag	UNP P59537
R	324	SER	-	expression tag	UNP P59537
R	325	GLY	-	expression tag	UNP P59537
R	326	GLY	-	expression tag	UNP P59537
R	327	GLY	-	expression tag	UNP P59537
R	328	GLY	-	expression tag	UNP P59537
R	329	SER	-	expression tag	UNP P59537
R	330	GLY	-	expression tag	UNP P59537
R	331	GLY	-	expression tag	UNP P59537
R	332	SER	-	expression tag	UNP P59537
R	333	SER	-	expression tag	UNP P59537
R	334	SER	-	expression tag	UNP P59537
R	335	GLY	-	expression tag	UNP P59537
R	336	GLY	-	expression tag	UNP P59537
R	337	VAL	-	expression tag	UNP P59537
R	338	PHE	-	expression tag	UNP P59537
R	339	THR	-	expression tag	UNP P59537
R	340	LEU	-	expression tag	UNP P59537
R	341	GLU	-	expression tag	UNP P59537
R	342	ASP	-	expression tag	UNP P59537
R	343	PHE	-	expression tag	UNP P59537
R	344	VAL	-	expression tag	UNP P59537
R	345	GLY	-	expression tag	UNP P59537
R	346	ASP	-	expression tag	UNP P59537
R	347	TRP	-	expression tag	UNP P59537
R	348	GLU	-	expression tag	UNP P59537
R	349	GLN	-	expression tag	UNP P59537
R	350	THR	-	expression tag	UNP P59537
R	351	ALA	-	expression tag	UNP P59537
R	352	ALA	-	expression tag	UNP P59537
R	353	TYR	-	expression tag	UNP P59537
R	354	ASN	-	expression tag	UNP P59537
R	355	LEU	-	expression tag	UNP P59537
R	356	ASP	-	expression tag	UNP P59537
R	357	GLN	-	expression tag	UNP P59537
R	358	VAL	-	expression tag	UNP P59537
R	359	LEU	-	expression tag	UNP P59537
R	360	GLU	-	expression tag	UNP P59537
R	361	GLN	-	expression tag	UNP P59537
R	362	GLY	-	expression tag	UNP P59537
R	363	GLY	-	expression tag	UNP P59537

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	364	VAL	-	expression tag	UNP P59537
R	365	SER	-	expression tag	UNP P59537
R	366	SER	-	expression tag	UNP P59537
R	367	LEU	-	expression tag	UNP P59537
R	368	LEU	-	expression tag	UNP P59537
R	369	GLN	-	expression tag	UNP P59537
R	370	ASN	-	expression tag	UNP P59537
R	371	LEU	-	expression tag	UNP P59537
R	372	ALA	-	expression tag	UNP P59537
R	373	VAL	-	expression tag	UNP P59537
R	374	SER	-	expression tag	UNP P59537
R	375	VAL	-	expression tag	UNP P59537
R	376	THR	-	expression tag	UNP P59537
R	377	PRO	-	expression tag	UNP P59537
R	378	ILE	-	expression tag	UNP P59537
R	379	GLN	-	expression tag	UNP P59537
R	380	ARG	-	expression tag	UNP P59537
R	381	ILE	-	expression tag	UNP P59537
R	382	VAL	-	expression tag	UNP P59537
R	383	ARG	-	expression tag	UNP P59537
R	384	SER	-	expression tag	UNP P59537
R	385	GLY	-	expression tag	UNP P59537
R	386	GLU	-	expression tag	UNP P59537
R	387	ASN	-	expression tag	UNP P59537
R	388	ALA	-	expression tag	UNP P59537
R	389	LEU	-	expression tag	UNP P59537
R	390	LYS	-	expression tag	UNP P59537
R	391	ILE	-	expression tag	UNP P59537
R	392	ASP	-	expression tag	UNP P59537
R	393	ILE	-	expression tag	UNP P59537
R	394	HIS	-	expression tag	UNP P59537
R	395	VAL	-	expression tag	UNP P59537
R	396	ILE	-	expression tag	UNP P59537
R	397	ILE	-	expression tag	UNP P59537
R	398	PRO	-	expression tag	UNP P59537
R	399	TYR	-	expression tag	UNP P59537
R	400	GLU	-	expression tag	UNP P59537
R	401	GLY	-	expression tag	UNP P59537
R	402	LEU	-	expression tag	UNP P59537
R	403	SER	-	expression tag	UNP P59537
R	404	ALA	-	expression tag	UNP P59537
R	405	ASP	-	expression tag	UNP P59537

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	406	GLN	-	expression tag	UNP P59537
R	407	MET	-	expression tag	UNP P59537
R	408	ALA	-	expression tag	UNP P59537
R	409	GLN	-	expression tag	UNP P59537
R	410	ILE	-	expression tag	UNP P59537
R	411	GLU	-	expression tag	UNP P59537
R	412	GLU	-	expression tag	UNP P59537
R	413	VAL	-	expression tag	UNP P59537
R	414	PHE	-	expression tag	UNP P59537
R	415	LYS	-	expression tag	UNP P59537
R	416	VAL	-	expression tag	UNP P59537
R	417	VAL	-	expression tag	UNP P59537
R	418	TYR	-	expression tag	UNP P59537
R	419	PRO	-	expression tag	UNP P59537
R	420	VAL	-	expression tag	UNP P59537
R	421	ASP	-	expression tag	UNP P59537
R	422	ASP	-	expression tag	UNP P59537
R	423	HIS	-	expression tag	UNP P59537
R	424	HIS	-	expression tag	UNP P59537
R	425	PHE	-	expression tag	UNP P59537
R	426	LYS	-	expression tag	UNP P59537
R	427	VAL	-	expression tag	UNP P59537
R	428	ILE	-	expression tag	UNP P59537
R	429	LEU	-	expression tag	UNP P59537
R	430	PRO	-	expression tag	UNP P59537
R	431	TYR	-	expression tag	UNP P59537
R	432	GLY	-	expression tag	UNP P59537
R	433	THR	-	expression tag	UNP P59537
R	434	LEU	-	expression tag	UNP P59537
R	435	VAL	-	expression tag	UNP P59537
R	436	ILE	-	expression tag	UNP P59537
R	437	ASP	-	expression tag	UNP P59537
R	438	GLY	-	expression tag	UNP P59537
R	439	VAL	-	expression tag	UNP P59537
R	440	THR	-	expression tag	UNP P59537
R	441	PRO	-	expression tag	UNP P59537
R	442	ASN	-	expression tag	UNP P59537
R	443	MET	-	expression tag	UNP P59537
R	444	LEU	-	expression tag	UNP P59537
R	445	ASN	-	expression tag	UNP P59537
R	446	TYR	-	expression tag	UNP P59537
R	447	PHE	-	expression tag	UNP P59537

Continued on next page...

Continued from previous page...

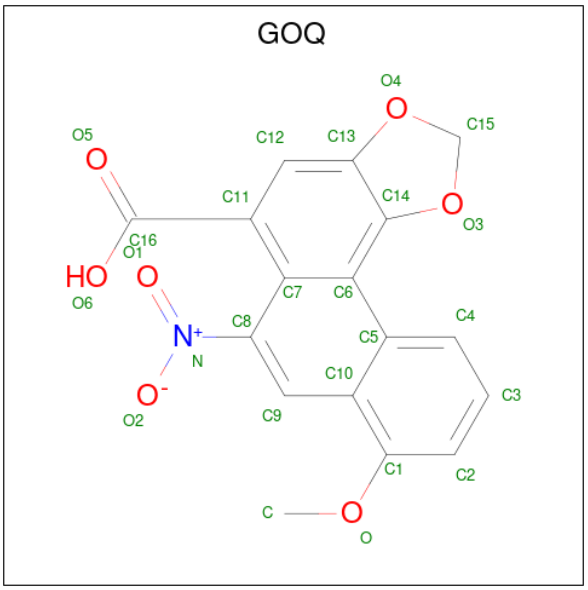
Chain	Residue	Modelled	Actual	Comment	Reference
R	448	GLY	-	expression tag	UNP P59537
R	449	ARG	-	expression tag	UNP P59537
R	450	PRO	-	expression tag	UNP P59537
R	451	TYR	-	expression tag	UNP P59537
R	452	GLU	-	expression tag	UNP P59537
R	453	GLY	-	expression tag	UNP P59537
R	454	ILE	-	expression tag	UNP P59537
R	455	ALA	-	expression tag	UNP P59537
R	456	VAL	-	expression tag	UNP P59537
R	457	PHE	-	expression tag	UNP P59537
R	458	ASP	-	expression tag	UNP P59537
R	459	GLY	-	expression tag	UNP P59537
R	460	LYS	-	expression tag	UNP P59537
R	461	LYS	-	expression tag	UNP P59537
R	462	ILE	-	expression tag	UNP P59537
R	463	THR	-	expression tag	UNP P59537
R	464	VAL	-	expression tag	UNP P59537
R	465	THR	-	expression tag	UNP P59537
R	466	GLY	-	expression tag	UNP P59537
R	467	THR	-	expression tag	UNP P59537
R	468	LEU	-	expression tag	UNP P59537
R	469	TRP	-	expression tag	UNP P59537
R	470	ASN	-	expression tag	UNP P59537
R	471	GLY	-	expression tag	UNP P59537
R	472	ASN	-	expression tag	UNP P59537
R	473	LYS	-	expression tag	UNP P59537
R	474	ILE	-	expression tag	UNP P59537
R	475	ILE	-	expression tag	UNP P59537
R	476	ASP	-	expression tag	UNP P59537
R	477	GLU	-	expression tag	UNP P59537
R	478	ARG	-	expression tag	UNP P59537
R	479	LEU	-	expression tag	UNP P59537
R	480	ILE	-	expression tag	UNP P59537
R	481	THR	-	expression tag	UNP P59537
R	482	PRO	-	expression tag	UNP P59537
R	483	ASP	-	expression tag	UNP P59537
R	484	GLY	-	expression tag	UNP P59537
R	485	SER	-	expression tag	UNP P59537
R	486	MET	-	expression tag	UNP P59537
R	487	LEU	-	expression tag	UNP P59537
R	488	PHE	-	expression tag	UNP P59537
R	489	ARG	-	expression tag	UNP P59537

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
R	490	VAL	-	expression tag	UNP P59537
R	491	THR	-	expression tag	UNP P59537
R	492	ILE	-	expression tag	UNP P59537
R	493	ASN	-	expression tag	UNP P59537
R	494	SER	-	expression tag	UNP P59537

- Molecule 6 is 8-methoxy-6-nitro-naphtho[1,2-e][1,3]benzodioxole-5-carboxylic acid (CCD ID: GOQ) (formula: $C_{17}H_{11}NO_7$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
6	R	1	Total	C	N	O	0
			25	17	1	7	

- Molecule 7 is water.

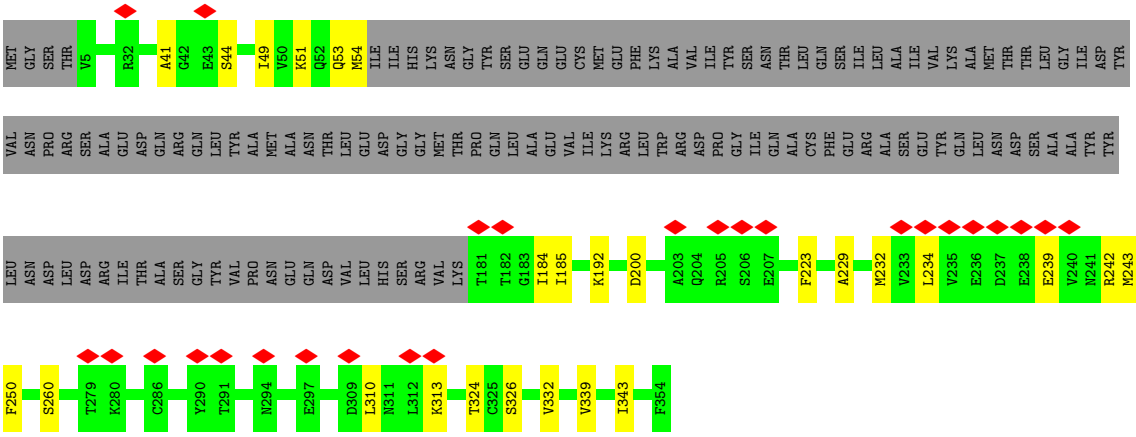
Mol	Chain	Residues	Atoms		AltConf
7	A	1	Total	O	0
			1	1	
7	R	4	Total	O	0
			4	4	

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.

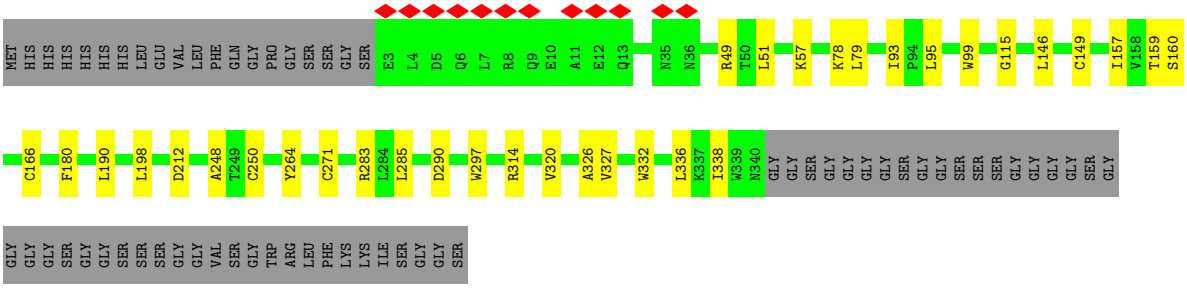
• Molecule 1: Guanine nucleotide-binding protein G(t) subunit alpha-3

Chain A:



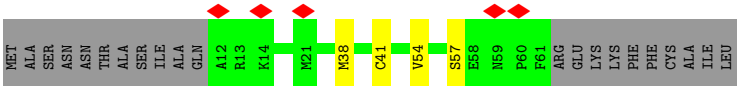
• Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



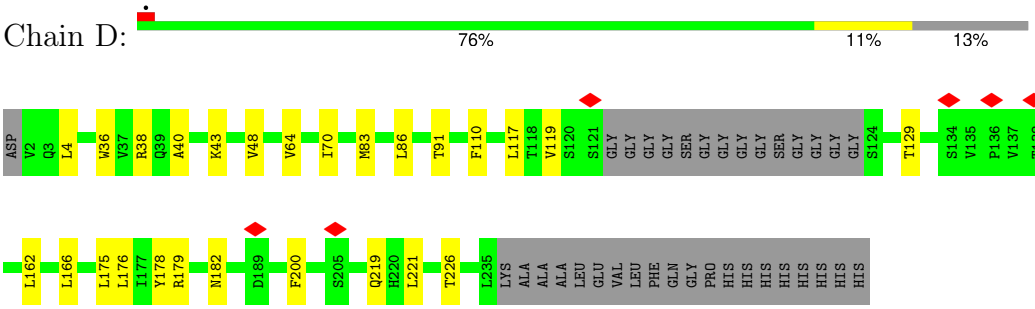
• Molecule 3: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

Chain C:



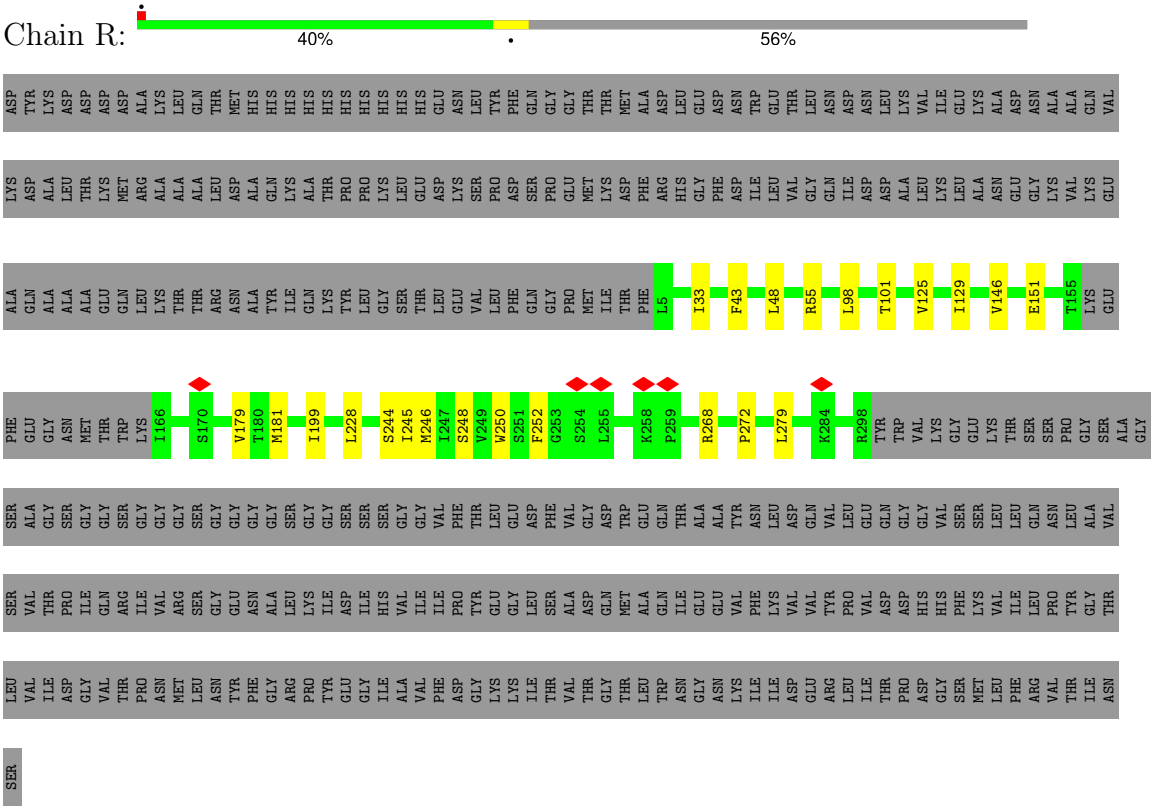
• Molecule 4: scFv16

Chain D:



• Molecule 5: Taste receptor type 2 member 43

Chain R:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	471455	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	20000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.967	Depositor
Minimum map value	-2.404	Depositor
Average map value	0.024	Depositor
Map value standard deviation	0.103	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	252.288, 252.288, 252.288	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.876, 0.876, 0.876	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOQ

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	0.14	0/1739	0.31	1/2341 (0.0%)
2	B	0.14	0/2504	0.30	0/3414
3	C	0.13	0/334	0.27	0/460
4	D	0.14	0/1805	0.29	0/2451
5	R	0.20	0/2304	0.33	0/3136
All	All	0.16	0/8686	0.31	1/11802 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	192	LYS	CB-CA-C	-5.26	110.08	117.23

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	1711	0	1643	15	0
2	B	2458	0	2271	22	0
3	C	328	0	291	3	0
4	D	1761	0	1685	17	0
5	R	2244	0	2323	22	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	R	25	0	0	2	0
7	A	1	0	0	0	0
7	R	4	0	0	2	0
All	All	8532	0	8213	76	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 (76) 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)
5:R:252:PHE:HE1	7:R:604:HOH:O	1.55	0.90
5:R:146:VAL:HG11	5:R:179:VAL:HG11	1.56	0.87
5:R:248:SER:HB2	5:R:268:ARG:HH22	1.46	0.80
5:R:151:GLU:OE2	7:R:601:HOH:O	2.01	0.77
5:R:248:SER:CB	5:R:268:ARG:HH22	2.02	0.72
4:D:40:ALA:HB3	4:D:43:LYS:HB2	1.71	0.72
2:B:115:GLY:HA3	2:B:146:LEU:HD23	1.73	0.70
4:D:91:THR:HG22	4:D:119:VAL:H	1.58	0.69
2:B:271:CYS:HB2	2:B:290:ASP:HB2	1.80	0.62
4:D:147:CYS:HB3	4:D:200:PHE:HB2	1.80	0.62
1:A:324:THR:HG22	1:A:326:SER:H	1.65	0.59
5:R:181:MET:HE1	5:R:250:TRP:HE3	1.67	0.59
5:R:55:ARG:HD3	5:R:272:PRO:HA	1.86	0.58
2:B:250:CYS:HB2	2:B:264:TYR:HB2	1.85	0.57
1:A:184:ILE:HD13	2:B:99:TRP:HD1	1.69	0.56
4:D:166:LEU:HB2	4:D:176:LEU:HD11	1.87	0.56
2:B:51:LEU:HB2	2:B:336:LEU:HB2	1.86	0.56
2:B:146:LEU:HD11	2:B:159:THR:HB	1.88	0.56
5:R:181:MET:HA	5:R:246:MET:HE1	1.89	0.55
2:B:248:ALA:HB2	2:B:271:CYS:H	1.72	0.55
1:A:234:LEU:HD23	1:A:239:GLU:HB2	1.89	0.53
3:C:54:VAL:HB	3:C:57:SER:HB2	1.89	0.53
1:A:232:MET:HB3	1:A:242:ARG:HD2	1.89	0.53
2:B:79:LEU:HB3	2:B:93:ILE:HB	1.91	0.53
1:A:184:ILE:HD13	2:B:99:TRP:CD1	2.45	0.52
2:B:320:VAL:HG22	2:B:327:VAL:HG22	1.92	0.50
5:R:101:THR:HG23	5:R:129:ILE:HD12	1.94	0.50
5:R:248:SER:HB2	5:R:268:ARG:NH2	2.23	0.50
5:R:43:PHE:HZ	5:R:129:ILE:HG21	1.78	0.49
4:D:36:TRP:HD1	4:D:70:ILE:HD12	1.77	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:ILE:HB	1:A:200:ASP:HB3	1.94	0.49
1:A:53:GLN:HG3	1:A:332:VAL:HG22	1.94	0.48
2:B:166:CYS:HB2	2:B:180:PHE:HB2	1.96	0.48
5:R:48:LEU:HD22	5:R:279:LEU:HD13	1.96	0.48
5:R:125:VAL:O	5:R:129:ILE:HG12	2.15	0.47
2:B:198:LEU:HD23	2:B:212:ASP:HA	1.97	0.46
4:D:48:VAL:HG13	4:D:64:VAL:HG21	1.97	0.46
4:D:38:ARG:HG3	4:D:48:VAL:HG21	1.97	0.45
2:B:49:ARG:HB2	2:B:338:ILE:HD13	1.99	0.45
2:B:79:LEU:HB2	2:B:95:LEU:HD21	1.98	0.45
1:A:41:ALA:HB3	1:A:44:SER:HB3	1.98	0.45
5:R:268:ARG:NH1	6:R:501:GOQ:O5	2.48	0.45
2:B:290:ASP:HA	2:B:314:ARG:HG3	1.99	0.45
5:R:245:ILE:HG22	5:R:246:MET:HE2	1.98	0.45
5:R:268:ARG:HH11	6:R:501:GOQ:C16	2.29	0.45
4:D:175:LEU:HD21	4:D:178:TYR:HB3	1.99	0.44
4:D:219:GLN:HE21	4:D:226:THR:H	1.66	0.44
4:D:83:MET:HE1	4:D:117:LEU:HD13	2.00	0.44
4:D:178:TYR:HD2	4:D:179:ARG:HE	1.65	0.44
2:B:57:LYS:HD2	2:B:332:TRP:CD2	2.52	0.43
2:B:78:LYS:HA	2:B:78:LYS:HD3	1.79	0.43
4:D:162:LEU:HD22	4:D:200:PHE:CG	2.53	0.43
1:A:250:PHE:HD2	1:A:310:LEU:HD23	1.83	0.43
4:D:153:LEU:HA	4:D:221:LEU:HD22	1.98	0.43
2:B:285:LEU:HB3	2:B:297:TRP:HB2	2.01	0.43
2:B:149:CYS:HB2	2:B:157:ILE:HD11	2.01	0.43
1:A:260:SER:HB2	1:A:313:LYS:HE3	2.01	0.43
5:R:244:SER:O	5:R:268:ARG:NH2	2.53	0.42
2:B:283:ARG:HB2	3:C:41:CYS:SG	2.59	0.42
5:R:199:ILE:HG23	5:R:228:LEU:HD11	2.00	0.42
5:R:98:LEU:HD23	5:R:98:LEU:HA	1.93	0.42
2:B:160:SER:HB3	2:B:190:LEU:HG	2.01	0.42
5:R:43:PHE:CZ	5:R:129:ILE:HG21	2.55	0.42
2:B:326:ALA:HB1	2:B:338:ILE:HG23	2.00	0.41
1:A:49:ILE:HG23	1:A:53:GLN:HE22	1.85	0.41
4:D:179:ARG:HB2	4:D:182:ASN:HD22	1.86	0.41
4:D:4:LEU:HD12	4:D:110:PHE:HD2	1.86	0.41
1:A:229:ALA:HB3	1:A:243:MET:HE2	2.00	0.41
4:D:83:MET:HB3	4:D:86:LEU:HD21	2.02	0.41
5:R:33:ILE:HD13	5:R:33:ILE:HA	1.90	0.41
1:A:339:VAL:O	1:A:343:ILE:HG12	2.21	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:51:LYS:HA	1:A:54:MET:HG2	2.03	0.41
4:D:129:THR:HB	4:D:148:ARG:HB2	2.03	0.41
3:C:38:MET:HE2	3:C:38:MET:HB3	1.86	0.40
1:A:223:PHE:HZ	1:A:249:LEU:HB3	1.86	0.40
5:R:244:SER:C	5:R:268:ARG:HH21	2.29	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	220/354 (62%)	210 (96%)	10 (4%)	0	100	100
2	B	336/402 (84%)	322 (96%)	14 (4%)	0	100	100
3	C	48/71 (68%)	45 (94%)	3 (6%)	0	100	100
4	D	228/267 (85%)	226 (99%)	2 (1%)	0	100	100
5	R	280/645 (43%)	268 (96%)	12 (4%)	0	100	100
All	All	1112/1739 (64%)	1071 (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	176/311 (57%)	176 (100%)	0	100	100
2	B	246/319 (77%)	246 (100%)	0	100	100
3	C	26/58 (45%)	26 (100%)	0	100	100
4	D	192/216 (89%)	192 (100%)	0	100	100
5	R	246/556 (44%)	246 (100%)	0	100	100
All	All	886/1460 (61%)	886 (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 (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	52	GLN
2	B	32	GLN
2	B	175	GLN
2	B	230	ASN
2	B	259	GLN
4	D	39	GLN
4	D	159	ASN
4	D	167	GLN
5	R	112	ASN
5	R	283	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)

1 ligand is 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	GOQ	R	501	-	28,28,28	0.95	2 (7%)	30,42,42	1.76	5 (16%)

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	GOQ	R	501	-	-	6/8/16/16	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	501	GOQ	O2-N	-2.12	1.21	1.35
6	R	501	GOQ	O6-C16	-2.08	1.24	1.30

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	501	GOQ	C8-C7-C6	-5.29	115.08	118.69
6	R	501	GOQ	C1-C10-C5	4.25	121.58	118.94
6	R	501	GOQ	C12-C11-C16	-3.16	112.34	117.67
6	R	501	GOQ	O5-C16-C11	-2.78	115.10	122.31
6	R	501	GOQ	O6-C16-O5	2.42	128.56	123.35

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	501	GOQ	C7-C8-N-O1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
6	R	501	GOQ	C9-C8-N-O1
6	R	501	GOQ	C12-C11-C16-O6
6	R	501	GOQ	C7-C11-C16-O5
6	R	501	GOQ	C7-C11-C16-O6
6	R	501	GOQ	C12-C11-C16-O5

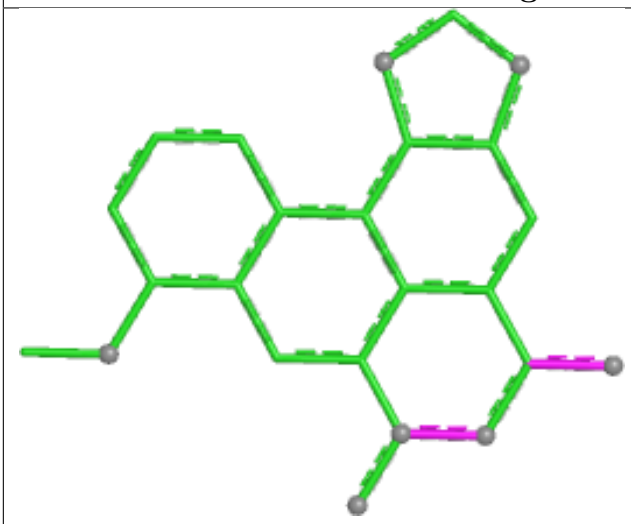
There are no ring outliers.

1 monomer is involved in 2 short contacts:

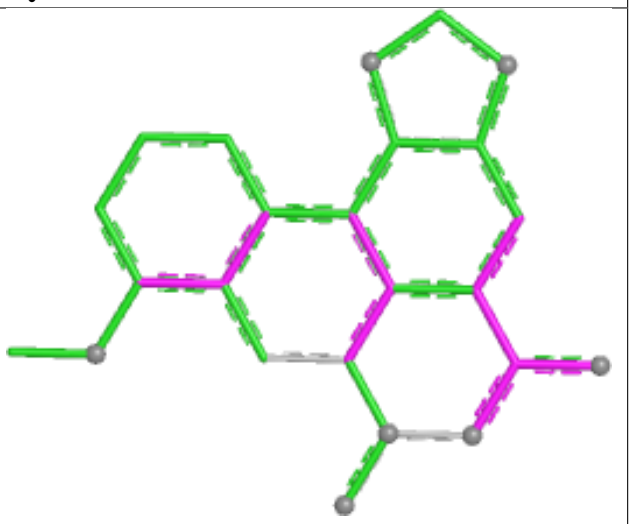
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	R	501	GOQ	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

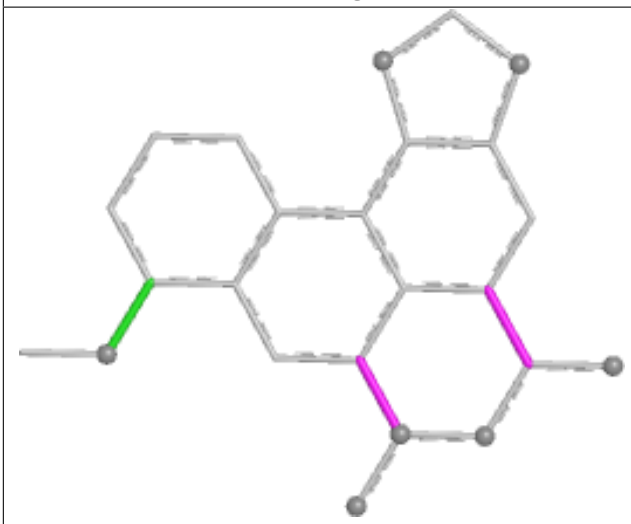
Ligand GOQ R 501



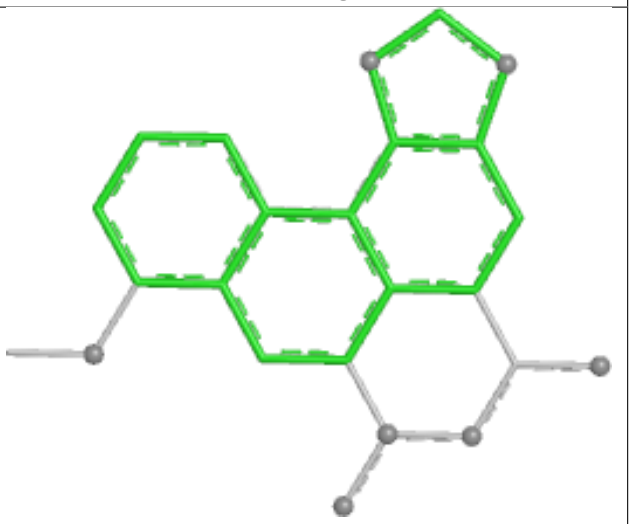
Bond lengths



Bond angles



Torsions



Rings

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.

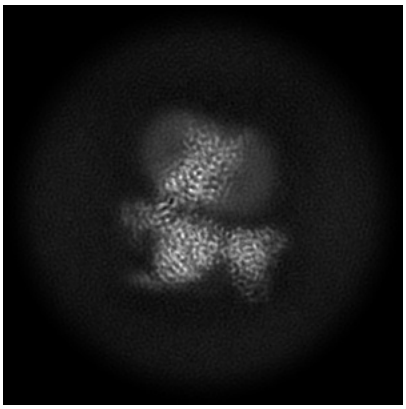
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-70965. These allow visual inspection of the internal detail of the map and identification of artifacts.

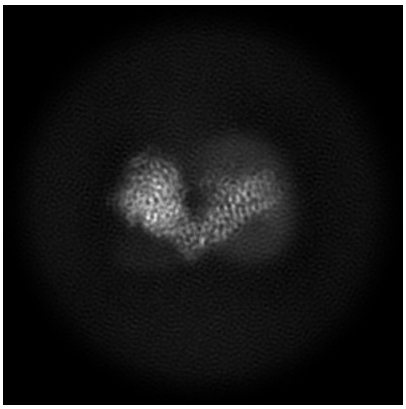
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

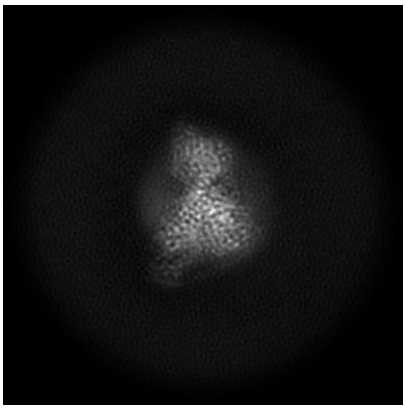
6.1.1 Primary map



X

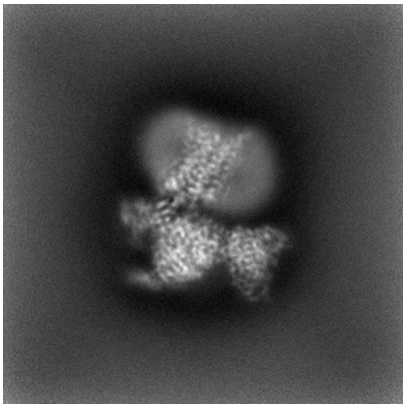


Y

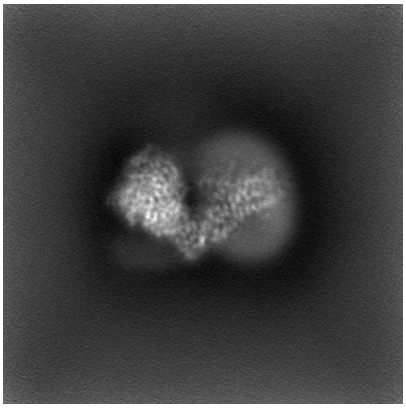


Z

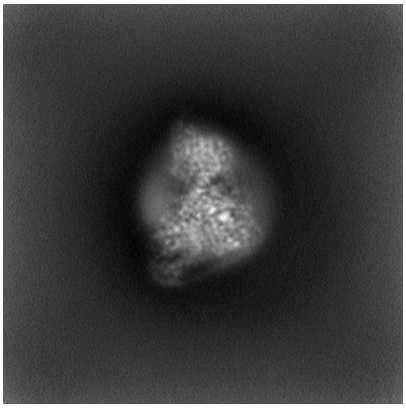
6.1.2 Raw map



X



Y

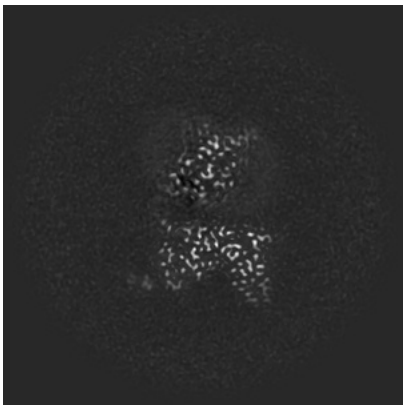


Z

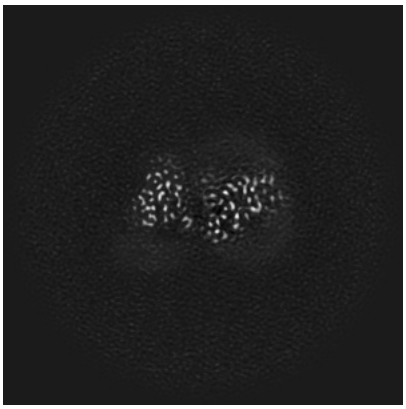
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

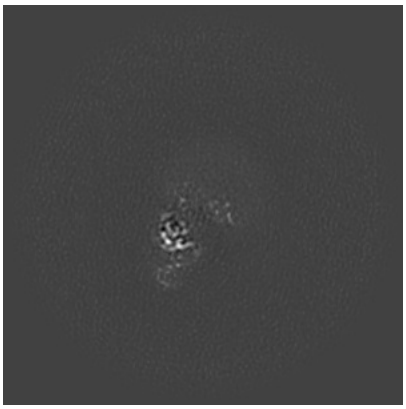
6.2.1 Primary map



X Index: 144

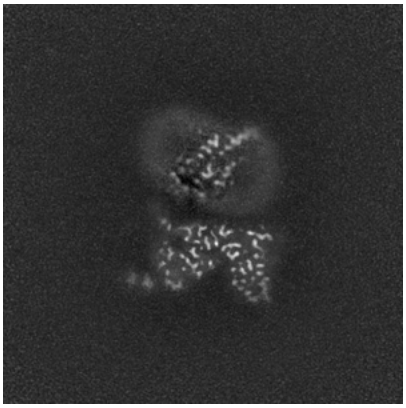


Y Index: 144

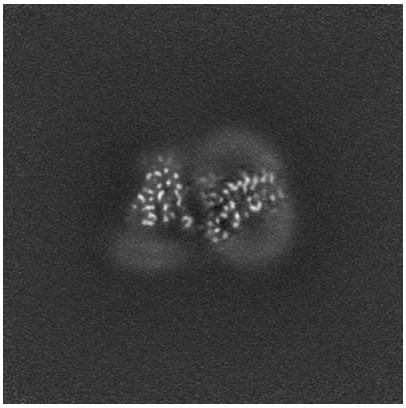


Z Index: 144

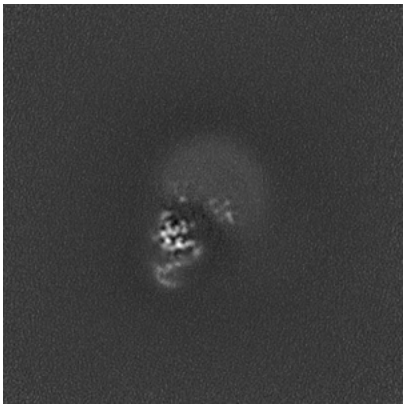
6.2.2 Raw map



X Index: 144



Y Index: 144

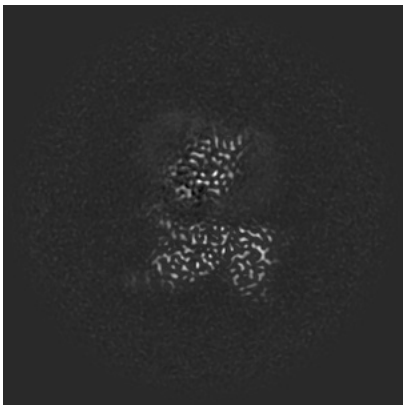


Z Index: 144

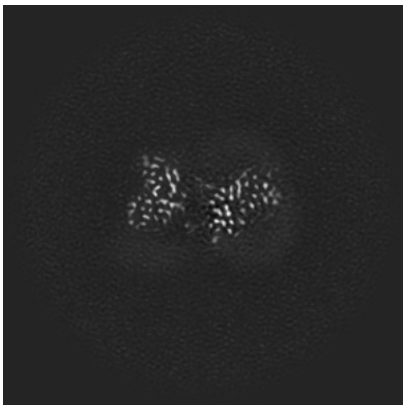
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

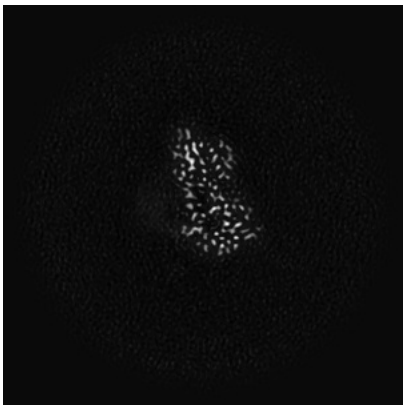
6.3.1 Primary map



X Index: 142

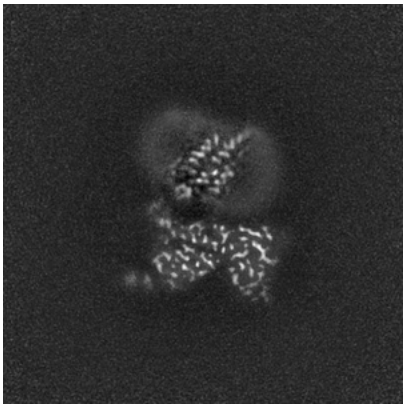


Y Index: 141

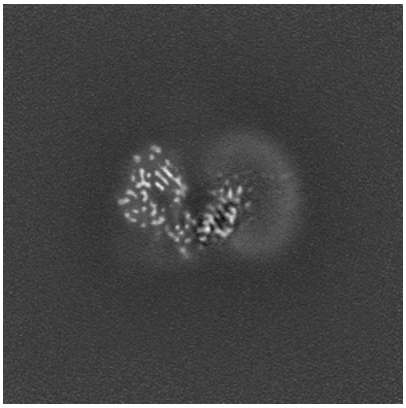


Z Index: 109

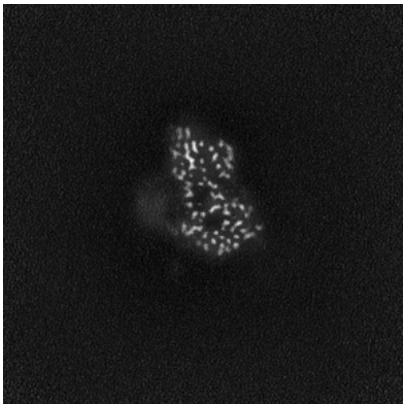
6.3.2 Raw map



X Index: 142



Y Index: 127

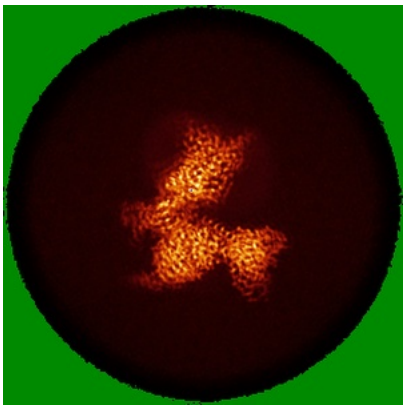


Z Index: 109

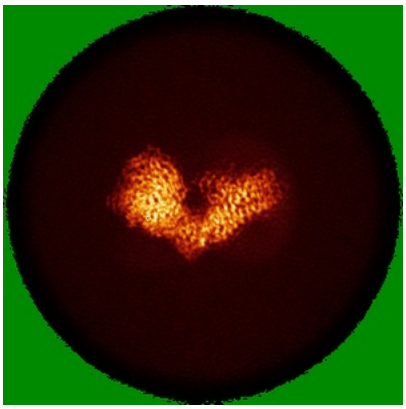
The images above show the largest variance slices of the map in three orthogonal directions.

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

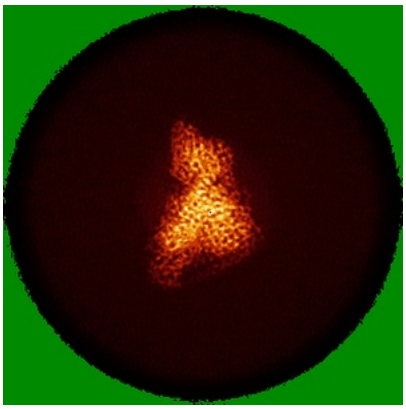
6.4.1 Primary map



X

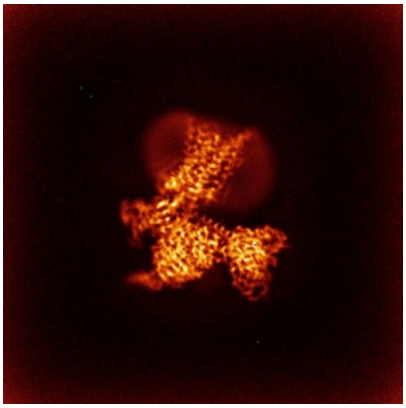


Y

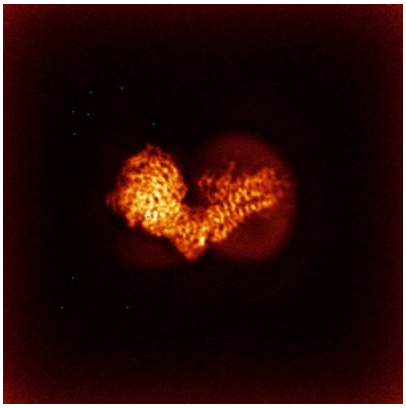


Z

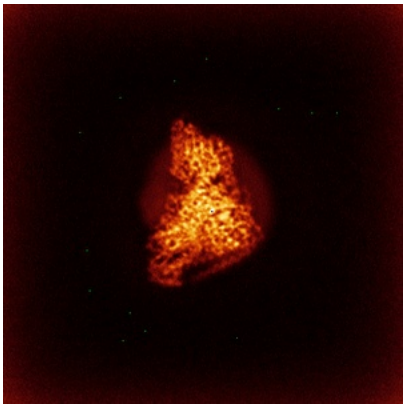
6.4.2 Raw map



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

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

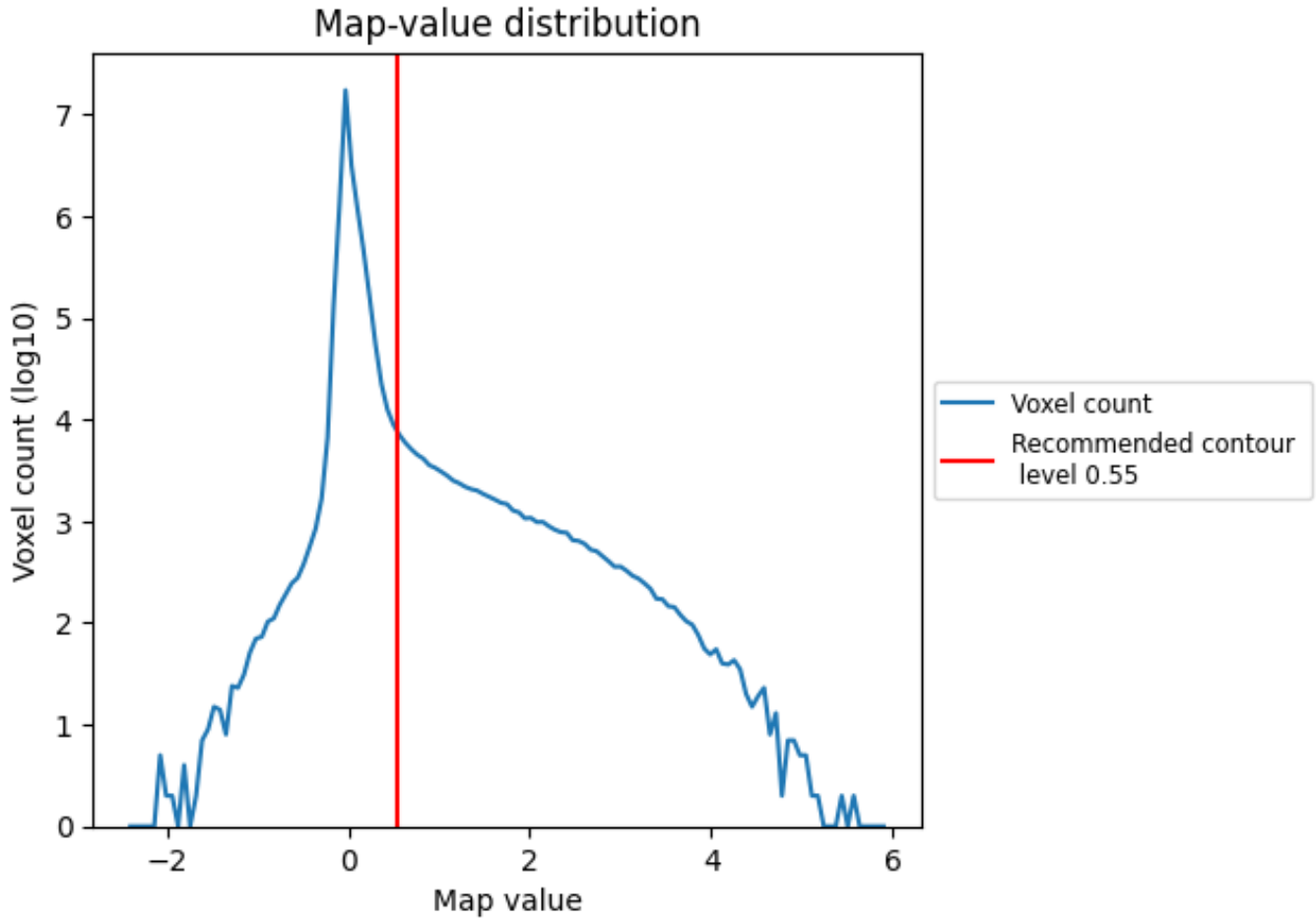
6.6 Mask visualisation (i)

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

7 Map analysis

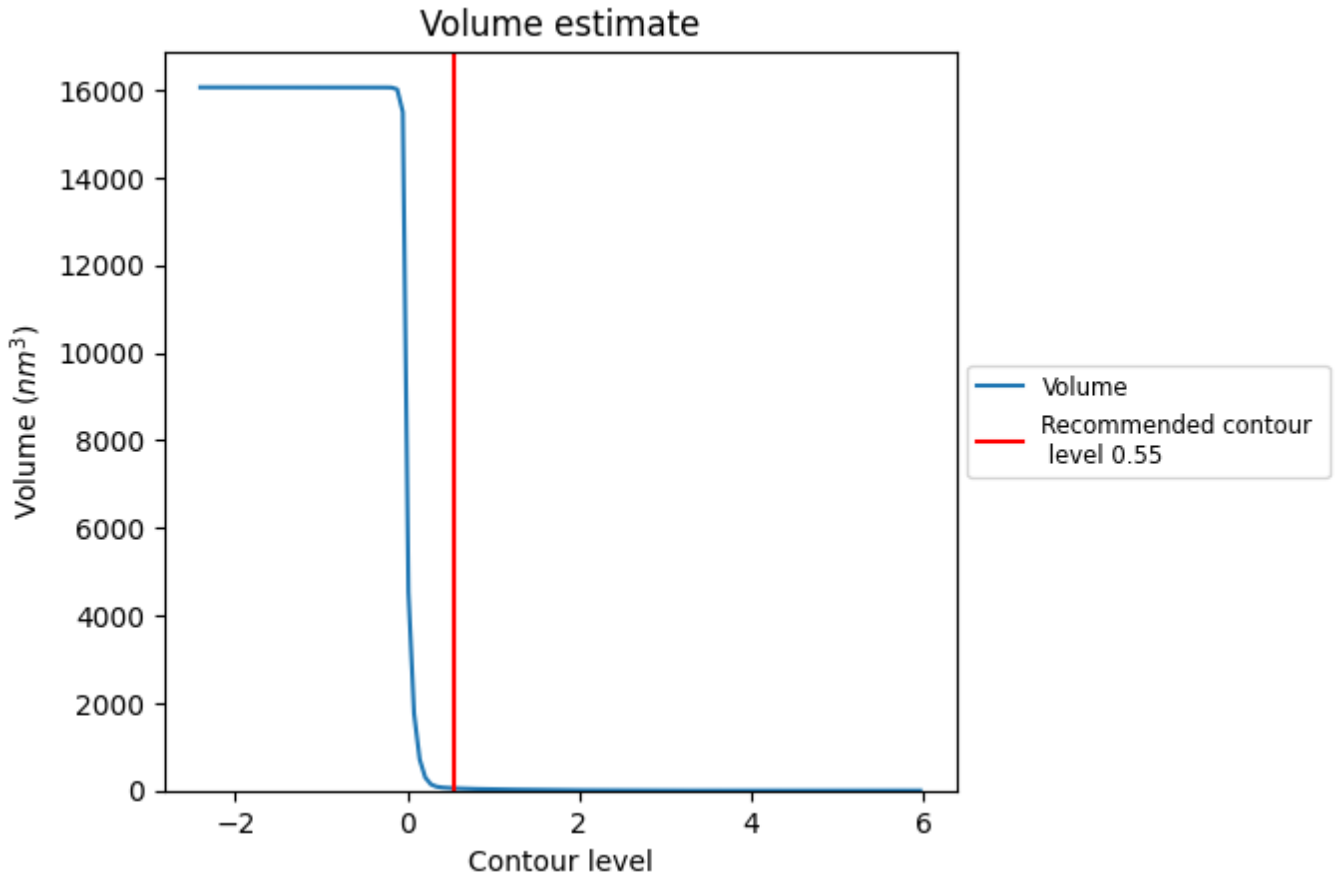
This section contains the results of statistical analysis of the map.

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.

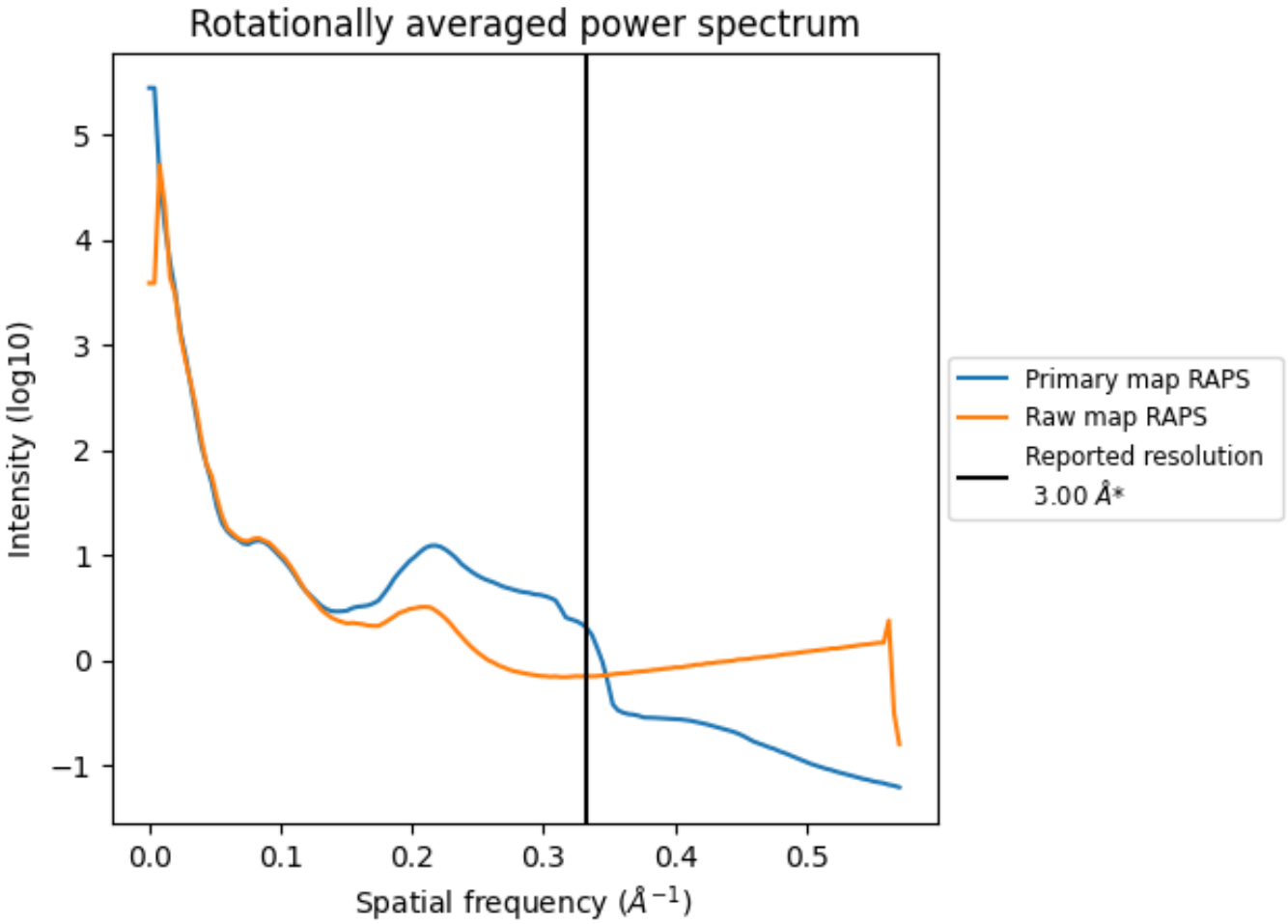
7.2 Volume estimate



The volume at the recommended contour level is 52 nm^3; this corresponds to an approximate mass of 47 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)

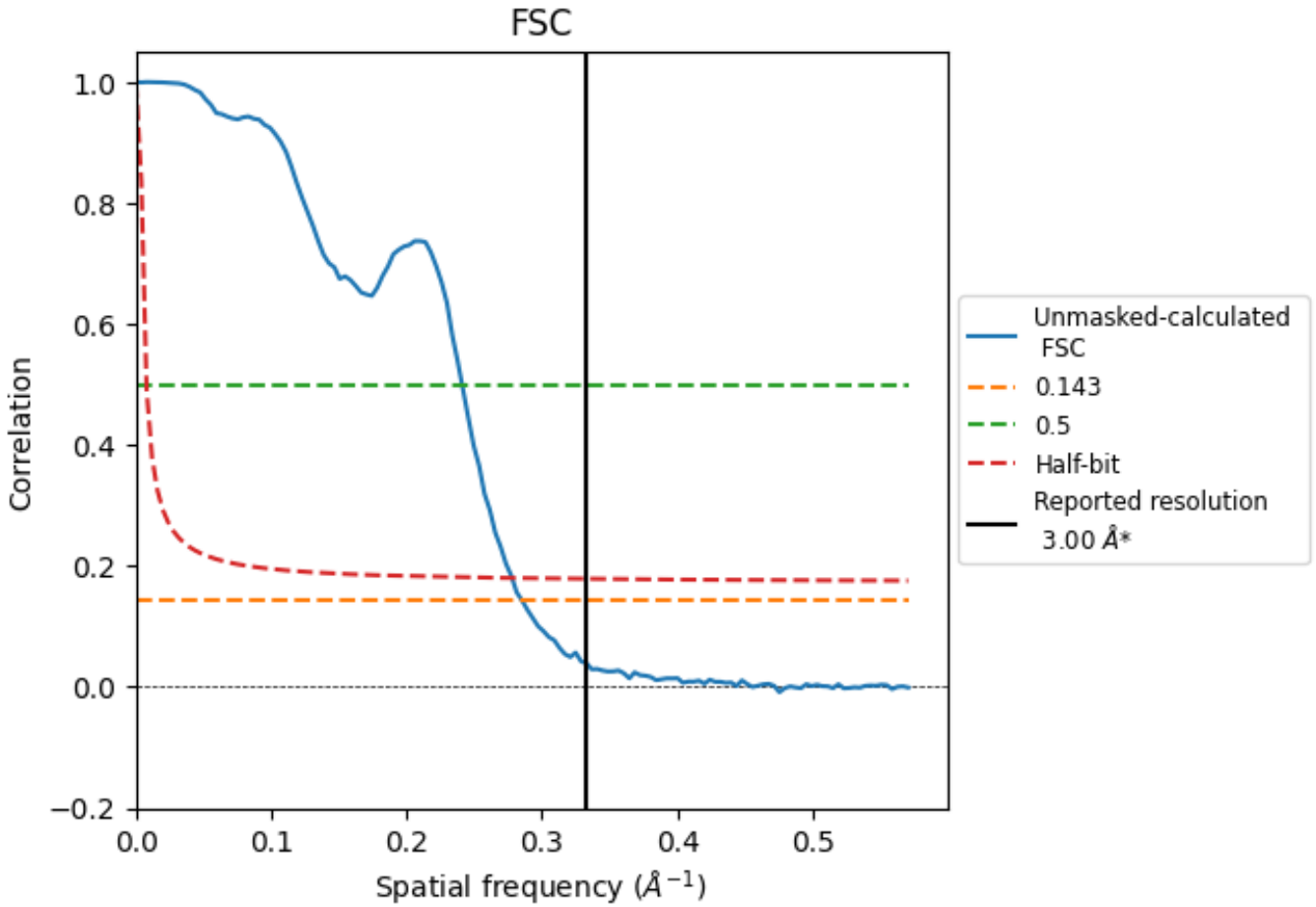


*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.333 Å^{-1}

8.2 Resolution estimates (i)

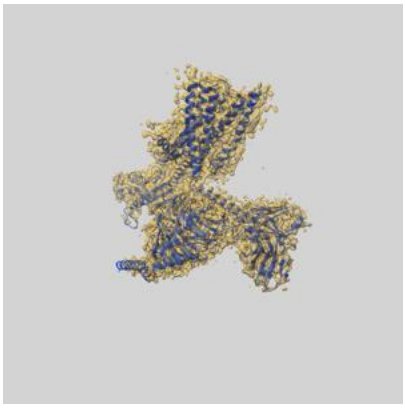
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.00	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.51	4.15	3.60

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.51 differs from the reported value 3.0 by more than 10 %

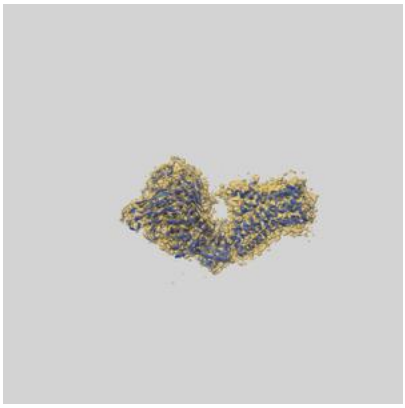
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-70965 and PDB model 9OXB. Per-residue inclusion information can be found in section 3 on page 16.

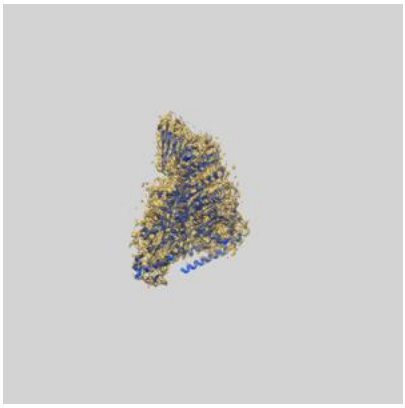
9.1 Map-model overlay



X



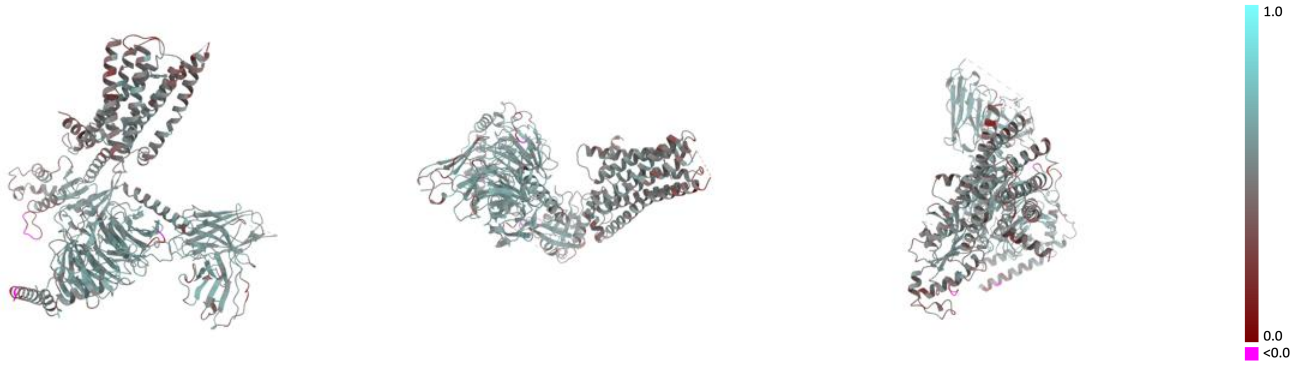
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55 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.

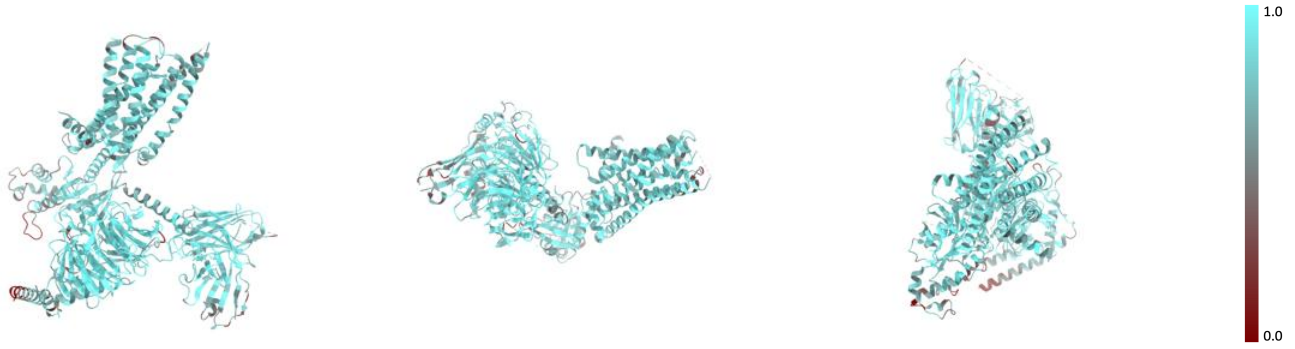
9.2 Q-score mapped to coordinate model (i)



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.

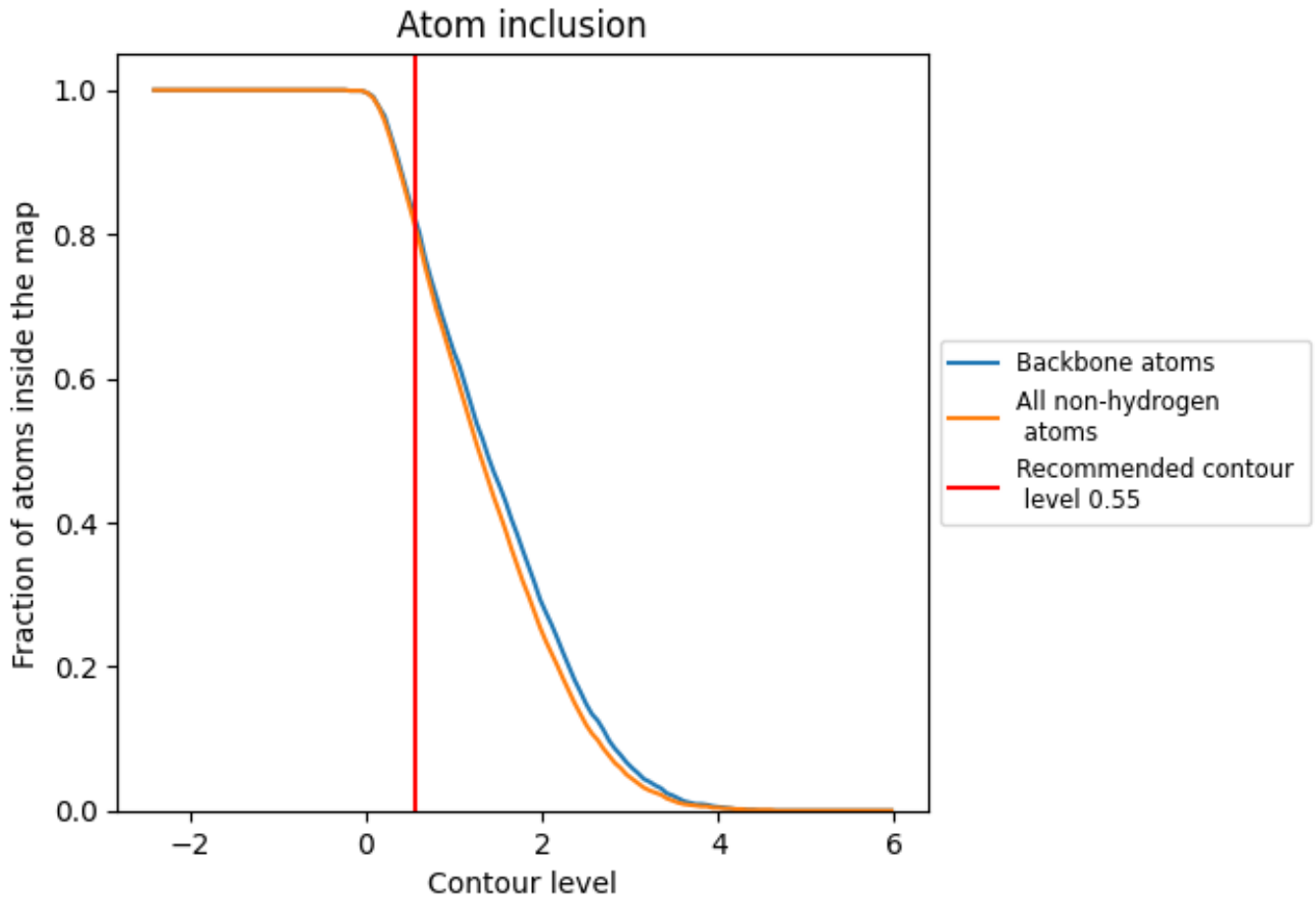
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.55).

9.4 Atom inclusion (i)



At the recommended contour level, 82% of all backbone atoms, 81% 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 (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8140	0.5150
A	0.7350	0.4700
B	0.8740	0.5670
C	0.7110	0.4820
D	0.8470	0.5550
R	0.8060	0.4660