wwPDB EM Validation Summary Report (i)

Oct 5, 2026 – 02:19 PM EDT

PDB ID	:	9YH3 / pdb_00009yh3
EMDB ID	:	EMD-72952
Title	:	Cis-azomorphine-3 bound mu opioid receptor Gi complex
Authors	:	Gati, C.; Khan, S.; Han, G.W.
Deposited on	:	2025-09-30
Resolution	:	3.29 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 (i) 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 (i)) were used in the production of this report:

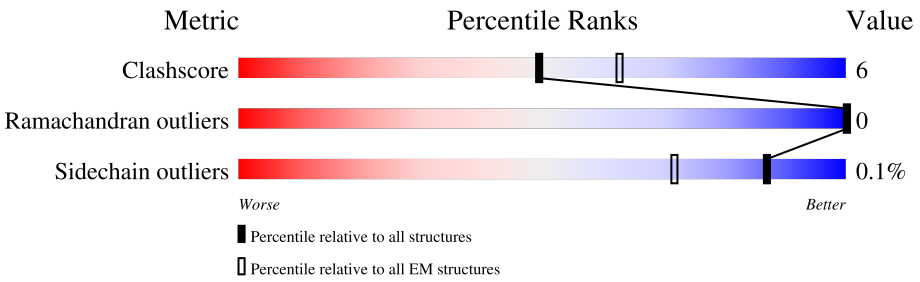
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.2
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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)	:	2.51

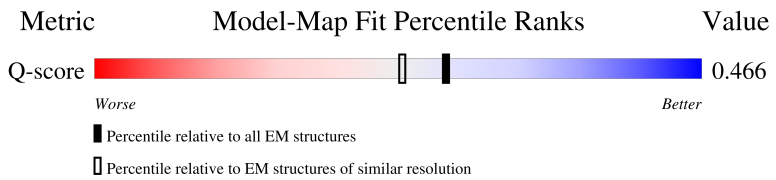
1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.29 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	14466 (2.79 - 3.79)

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	B	361	• 75% 18% 7%
2	C	71	• 63% 11% 25%
3	R	622	6% 38% 8% 54%
4	A	354	• 58% • 38%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 7089 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(I)/G(S)/G(T) subunit beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	336	2547	1577	458	493	19	0	0

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-20	HIS	-	expression tag	UNP P62873
B	-19	HIS	-	expression tag	UNP P62873
B	-18	HIS	-	expression tag	UNP P62873
B	-17	HIS	-	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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	53	381	243	67	68	3	0	0

- Molecule 3 is a protein called Mu-type opioid receptor.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	R	287	2309	1533	368	383	25	0	0

There are 223 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	-169	MET	-	initiating methionine	UNP P35372
R	-168	LYS	-	expression tag	UNP P35372
R	-167	THR	-	expression tag	UNP P35372
R	-166	ILE	-	expression tag	UNP P35372
R	-165	ILE	-	expression tag	UNP P35372
R	-164	ALA	-	expression tag	UNP P35372
R	-163	LEU	-	expression tag	UNP P35372
R	-162	SER	-	expression tag	UNP P35372
R	-161	TYR	-	expression tag	UNP P35372
R	-160	ILE	-	expression tag	UNP P35372
R	-159	PHE	-	expression tag	UNP P35372
R	-158	CYS	-	expression tag	UNP P35372
R	-157	LEU	-	expression tag	UNP P35372
R	-156	VAL	-	expression tag	UNP P35372
R	-155	PHE	-	expression tag	UNP P35372
R	-154	ALA	-	expression tag	UNP P35372
R	-153	ASP	-	expression tag	UNP P35372
R	-152	TYR	-	expression tag	UNP P35372
R	-151	LYS	-	expression tag	UNP P35372
R	-150	ASP	-	expression tag	UNP P35372
R	-149	HIS	-	expression tag	UNP P35372
R	-148	ASP	-	expression tag	UNP P35372
R	-147	GLY	-	expression tag	UNP P35372
R	-146	ASP	-	expression tag	UNP P35372
R	-145	TYR	-	expression tag	UNP P35372
R	-144	LYS	-	expression tag	UNP P35372
R	-143	ASP	-	expression tag	UNP P35372
R	-142	HIS	-	expression tag	UNP P35372
R	-141	ASP	-	expression tag	UNP P35372
R	-140	ILE	-	expression tag	UNP P35372
R	-139	ASP	-	expression tag	UNP P35372

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-138	TYR	-	expression tag	UNP P35372
R	-137	LYS	-	expression tag	UNP P35372
R	-136	ASP	-	expression tag	UNP P35372
R	-135	ASP	-	expression tag	UNP P35372
R	-134	ASP	-	expression tag	UNP P35372
R	-133	ASP	-	expression tag	UNP P35372
R	-132	LYS	-	expression tag	UNP P35372
R	-131	LEU	-	expression tag	UNP P35372
R	-130	HIS	-	expression tag	UNP P35372
R	-129	HIS	-	expression tag	UNP P35372
R	-128	HIS	-	expression tag	UNP P35372
R	-127	HIS	-	expression tag	UNP P35372
R	-126	HIS	-	expression tag	UNP P35372
R	-125	HIS	-	expression tag	UNP P35372
R	-124	HIS	-	expression tag	UNP P35372
R	-123	HIS	-	expression tag	UNP P35372
R	-122	HIS	-	expression tag	UNP P35372
R	-121	HIS	-	expression tag	UNP P35372
R	-120	LEU	-	expression tag	UNP P35372
R	-119	GLU	-	expression tag	UNP P35372
R	-118	VAL	-	expression tag	UNP P35372
R	-117	LEU	-	expression tag	UNP P35372
R	-116	PHE	-	expression tag	UNP P35372
R	-115	GLN	-	expression tag	UNP P35372
R	-114	GLY	-	expression tag	UNP P35372
R	-113	PRO	-	expression tag	UNP P35372
R	-112	GLY	-	expression tag	UNP P35372
R	-111	SER	-	expression tag	UNP P35372
R	-110	GLY	-	expression tag	UNP P35372
R	-109	SER	-	expression tag	UNP P35372
R	-108	ALA	-	expression tag	UNP P35372
R	-107	ASP	-	expression tag	UNP P35372
R	-106	LEU	-	expression tag	UNP P35372
R	-105	GLU	-	expression tag	UNP P35372
R	-104	ASP	-	expression tag	UNP P35372
R	-103	ASN	-	expression tag	UNP P35372
R	-102	TRP	-	expression tag	UNP P35372
R	-101	GLU	-	expression tag	UNP P35372
R	-100	THR	-	expression tag	UNP P35372
R	-99	LEU	-	expression tag	UNP P35372
R	-98	ASN	-	expression tag	UNP P35372
R	-97	ASP	-	expression tag	UNP P35372

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-96	ASN	-	expression tag	UNP P35372
R	-95	LEU	-	expression tag	UNP P35372
R	-94	LYS	-	expression tag	UNP P35372
R	-93	VAL	-	expression tag	UNP P35372
R	-92	ILE	-	expression tag	UNP P35372
R	-91	GLU	-	expression tag	UNP P35372
R	-90	LYS	-	expression tag	UNP P35372
R	-89	ALA	-	expression tag	UNP P35372
R	-88	ASP	-	expression tag	UNP P35372
R	-87	ASN	-	expression tag	UNP P35372
R	-86	ALA	-	expression tag	UNP P35372
R	-85	ALA	-	expression tag	UNP P35372
R	-84	GLN	-	expression tag	UNP P35372
R	-83	VAL	-	expression tag	UNP P35372
R	-82	LYS	-	expression tag	UNP P35372
R	-81	ASP	-	expression tag	UNP P35372
R	-80	ALA	-	expression tag	UNP P35372
R	-79	LEU	-	expression tag	UNP P35372
R	-78	THR	-	expression tag	UNP P35372
R	-77	LYS	-	expression tag	UNP P35372
R	-76	MET	-	expression tag	UNP P35372
R	-75	ARG	-	expression tag	UNP P35372
R	-74	ALA	-	expression tag	UNP P35372
R	-73	ALA	-	expression tag	UNP P35372
R	-72	ALA	-	expression tag	UNP P35372
R	-71	LEU	-	expression tag	UNP P35372
R	-70	ASP	-	expression tag	UNP P35372
R	-69	ALA	-	expression tag	UNP P35372
R	-68	GLN	-	expression tag	UNP P35372
R	-67	LYS	-	expression tag	UNP P35372
R	-66	ALA	-	expression tag	UNP P35372
R	-65	THR	-	expression tag	UNP P35372
R	-64	PRO	-	expression tag	UNP P35372
R	-63	PRO	-	expression tag	UNP P35372
R	-62	LYS	-	expression tag	UNP P35372
R	-61	LEU	-	expression tag	UNP P35372
R	-60	GLU	-	expression tag	UNP P35372
R	-59	ASP	-	expression tag	UNP P35372
R	-58	LYS	-	expression tag	UNP P35372
R	-57	SER	-	expression tag	UNP P35372
R	-56	PRO	-	expression tag	UNP P35372
R	-55	ASP	-	expression tag	UNP P35372

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-54	SER	-	expression tag	UNP P35372
R	-53	PRO	-	expression tag	UNP P35372
R	-52	GLU	-	expression tag	UNP P35372
R	-51	MET	-	expression tag	UNP P35372
R	-50	LYS	-	expression tag	UNP P35372
R	-49	ASP	-	expression tag	UNP P35372
R	-48	PHE	-	expression tag	UNP P35372
R	-47	ARG	-	expression tag	UNP P35372
R	-46	HIS	-	expression tag	UNP P35372
R	-45	GLY	-	expression tag	UNP P35372
R	-44	PHE	-	expression tag	UNP P35372
R	-43	ASP	-	expression tag	UNP P35372
R	-42	ILE	-	expression tag	UNP P35372
R	-41	LEU	-	expression tag	UNP P35372
R	-40	VAL	-	expression tag	UNP P35372
R	-39	GLY	-	expression tag	UNP P35372
R	-38	GLN	-	expression tag	UNP P35372
R	-37	ILE	-	expression tag	UNP P35372
R	-36	ASP	-	expression tag	UNP P35372
R	-35	ASP	-	expression tag	UNP P35372
R	-34	ALA	-	expression tag	UNP P35372
R	-33	LEU	-	expression tag	UNP P35372
R	-32	LYS	-	expression tag	UNP P35372
R	-31	LEU	-	expression tag	UNP P35372
R	-30	ALA	-	expression tag	UNP P35372
R	-29	ASN	-	expression tag	UNP P35372
R	-28	GLU	-	expression tag	UNP P35372
R	-27	GLY	-	expression tag	UNP P35372
R	-26	LYS	-	expression tag	UNP P35372
R	-25	VAL	-	expression tag	UNP P35372
R	-24	LYS	-	expression tag	UNP P35372
R	-23	GLU	-	expression tag	UNP P35372
R	-22	ALA	-	expression tag	UNP P35372
R	-21	GLN	-	expression tag	UNP P35372
R	-20	ALA	-	expression tag	UNP P35372
R	-19	ALA	-	expression tag	UNP P35372
R	-18	ALA	-	expression tag	UNP P35372
R	-17	GLU	-	expression tag	UNP P35372
R	-16	GLN	-	expression tag	UNP P35372
R	-15	LEU	-	expression tag	UNP P35372
R	-14	LYS	-	expression tag	UNP P35372
R	-13	THR	-	expression tag	UNP P35372

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Chain	Residue	Modelled	Actual	Comment	Reference
R	-12	THR	-	expression tag	UNP P35372
R	-11	ARG	-	expression tag	UNP P35372
R	-10	ASN	-	expression tag	UNP P35372
R	-9	ALA	-	expression tag	UNP P35372
R	-8	TYR	-	expression tag	UNP P35372
R	-7	ILE	-	expression tag	UNP P35372
R	-6	GLN	-	expression tag	UNP P35372
R	-5	LYS	-	expression tag	UNP P35372
R	-4	TYR	-	expression tag	UNP P35372
R	-3	LEU	-	expression tag	UNP P35372
R	-2	GLY	-	expression tag	UNP P35372
R	-1	THR	-	expression tag	UNP P35372
R	0	GLY	-	expression tag	UNP P35372
R	1	SER	-	expression tag	UNP P35372
R	401	ALA	-	expression tag	UNP P35372
R	402	ALA	-	expression tag	UNP P35372
R	403	ALA	-	expression tag	UNP P35372
R	404	LEU	-	expression tag	UNP P35372
R	405	GLU	-	expression tag	UNP P35372
R	406	VAL	-	expression tag	UNP P35372
R	407	LEU	-	expression tag	UNP P35372
R	408	PHE	-	expression tag	UNP P35372
R	409	GLN	-	expression tag	UNP P35372
R	410	GLY	-	expression tag	UNP P35372
R	411	PRO	-	expression tag	UNP P35372
R	412	GLY	-	expression tag	UNP P35372
R	413	SER	-	expression tag	UNP P35372
R	414	TRP	-	expression tag	UNP P35372
R	415	SER	-	expression tag	UNP P35372
R	416	HIS	-	expression tag	UNP P35372
R	417	PRO	-	expression tag	UNP P35372
R	418	GLN	-	expression tag	UNP P35372
R	419	PHE	-	expression tag	UNP P35372
R	420	GLU	-	expression tag	UNP P35372
R	421	LYS	-	expression tag	UNP P35372
R	422	GLY	-	expression tag	UNP P35372
R	423	GLY	-	expression tag	UNP P35372
R	424	GLY	-	expression tag	UNP P35372
R	425	SER	-	expression tag	UNP P35372
R	426	GLY	-	expression tag	UNP P35372
R	427	GLY	-	expression tag	UNP P35372
R	428	GLY	-	expression tag	UNP P35372

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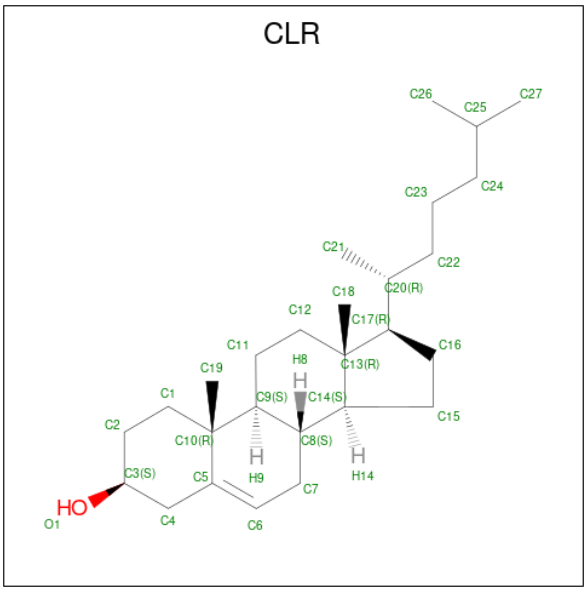
Chain	Residue	Modelled	Actual	Comment	Reference
R	429	SER	-	expression tag	UNP P35372
R	430	GLY	-	expression tag	UNP P35372
R	431	GLY	-	expression tag	UNP P35372
R	432	SER	-	expression tag	UNP P35372
R	433	SER	-	expression tag	UNP P35372
R	434	ALA	-	expression tag	UNP P35372
R	435	TRP	-	expression tag	UNP P35372
R	436	SER	-	expression tag	UNP P35372
R	437	HIS	-	expression tag	UNP P35372
R	438	PRO	-	expression tag	UNP P35372
R	439	GLN	-	expression tag	UNP P35372
R	440	PHE	-	expression tag	UNP P35372
R	441	GLU	-	expression tag	UNP P35372
R	442	LYS	-	expression tag	UNP P35372
R	443	HIS	-	expression tag	UNP P35372
R	444	HIS	-	expression tag	UNP P35372
R	445	HIS	-	expression tag	UNP P35372
R	446	HIS	-	expression tag	UNP P35372
R	447	HIS	-	expression tag	UNP P35372
R	448	HIS	-	expression tag	UNP P35372
R	449	HIS	-	expression tag	UNP P35372
R	450	HIS	-	expression tag	UNP P35372
R	451	HIS	-	expression tag	UNP P35372
R	452	HIS	-	expression tag	UNP P35372

- Molecule 4 is a protein called Guanine nucleotide-binding protein G(i) subunit alpha-1.

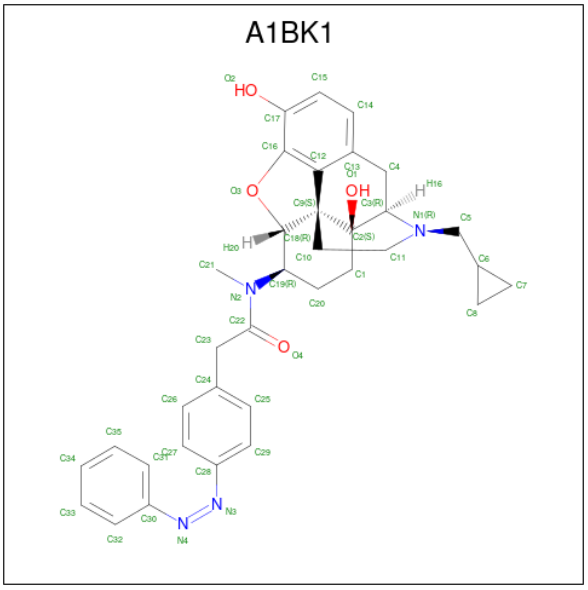
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	A	220	1725	1100	291	321	13	0	0

- Molecule 5 is CHOLESTEROL (CCD ID: CLR) (formula: $C_{27}H_{46}O$).



Mol	Chain	Residues	Atoms			AltConf
			Total	C	O	
5	R	1	28	27	1	0
			Total	C	O	
5	R	1	28	27	1	0
			Total	C	O	
5	R	1	28	27	1	0

- Molecule 6 is N-[17-(cyclopropylmethyl)-3,14-dihydroxy-5alpha-4,5-epoxymorphinan-6beta-yl]-N-methyl-2-{4-[(Z)-phenyldiazenyl]phenyl}acetamide (CCD ID: A1BK1) (formula: $C_{35}H_{38}N_4O_4$) (labeled as "Ligand of Interest" by depositor).



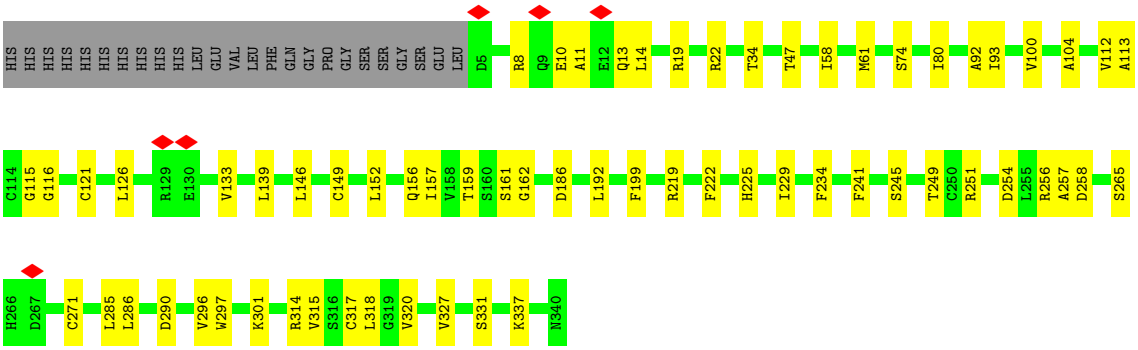
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
6	R	1	43	35	4	4	0

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.

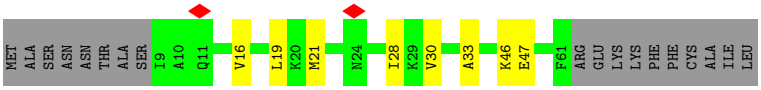
- Molecule 1: Guanine nucleotide-binding protein G(I)/G(S)/G(T) subunit beta-1

Chain B:



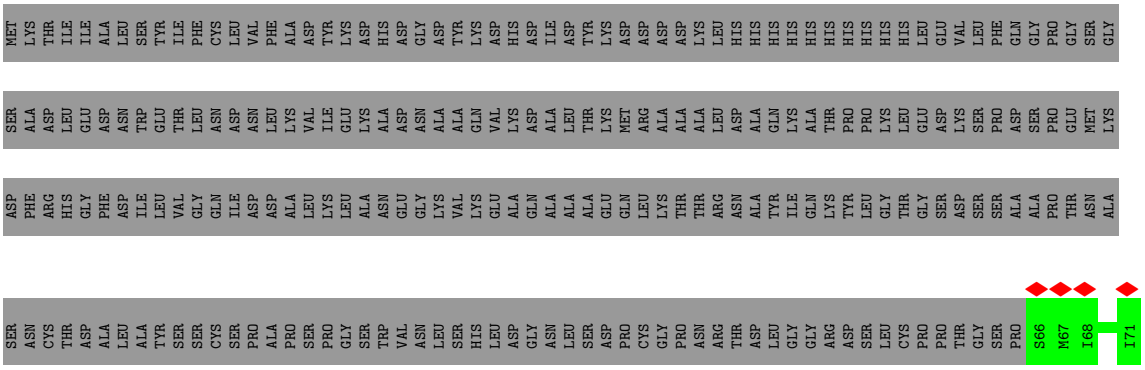
- Molecule 2: Guanine nucleotide-binding protein G(I)/G(S)/G(O) subunit gamma-2

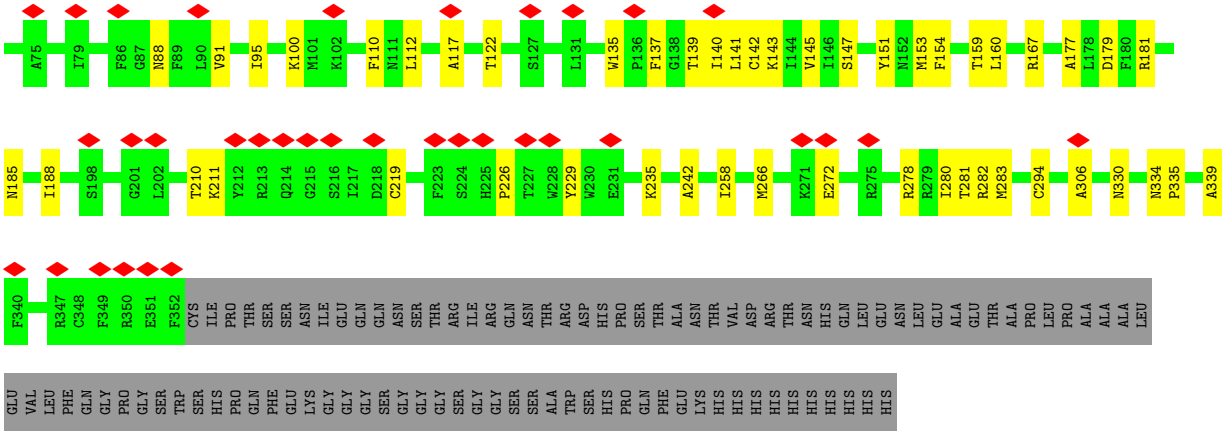
Chain C:



- Molecule 3: Mu-type opioid receptor

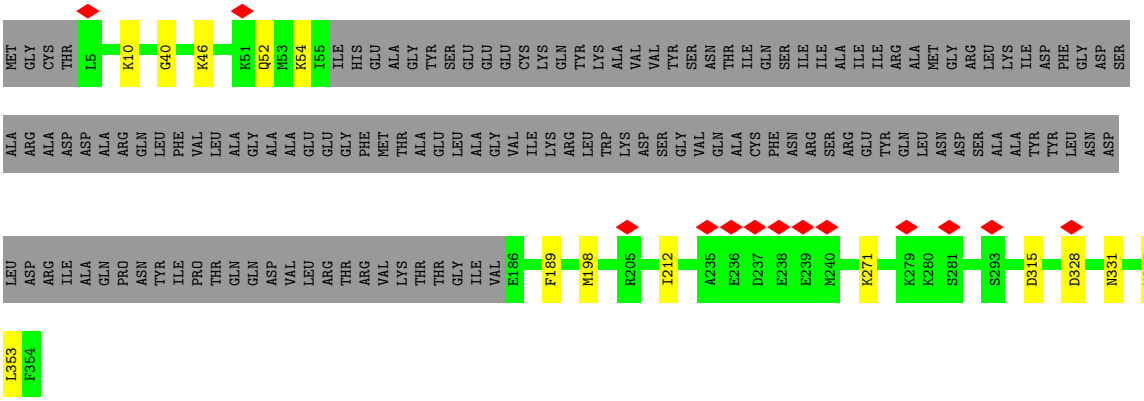
Chain R:





- Molecule 4: Guanine nucleotide-binding protein G(i) subunit alpha-1

Chain A:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	191338	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	130000	Depositor
Image detector	GATAN K3 BIOCONTINUUM (6k x 4k)	Depositor
Maximum map value	2.791	Depositor
Minimum map value	-1.646	Depositor
Average map value	0.008	Depositor
Map value standard deviation	0.037	Depositor
Recommended contour level	0.295	Depositor
Map size (Å)	331.264, 331.264, 331.264	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.294, 1.294, 1.294	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: CLR, A1BK1

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	B	0.18	0/2594	0.45	0/3520
2	C	0.11	0/387	0.30	0/527
3	R	0.20	0/2368	0.41	0/3225
4	A	0.15	0/1755	0.38	0/2359
All	All	0.17	0/7104	0.41	0/9631

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 (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2547	0	2437	40	0
2	C	381	0	378	7	0
3	R	2309	0	2400	30	0
4	A	1725	0	1676	11	0
5	R	84	0	138	2	0
6	R	43	0	0	0	0
All	All	7089	0	7029	81	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 6.

The worst 5 of 81 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:R:226:PRO:HB2	3:R:229:TYR:HB3	1.74	0.68
3:R:137:PHE:HB3	3:R:141:LEU:HD23	1.77	0.67
3:R:95:ILE:HG21	3:R:110:PHE:HB2	1.77	0.66
1:B:271:CYS:HB2	1:B:290:ASP:HB2	1.78	0.66
3:R:335:PRO:O	3:R:339:ALA:HB3	1.95	0.66

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	B	334/361 (92%)	316 (95%)	18 (5%)	0	100	100
2	C	51/71 (72%)	48 (94%)	3 (6%)	0	100	100
3	R	285/622 (46%)	279 (98%)	6 (2%)	0	100	100
4	A	216/354 (61%)	204 (94%)	12 (6%)	0	100	100
All	All	886/1408 (63%)	847 (96%)	39 (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	B	268/301 (89%)	268 (100%)	0	100	100
2	C	36/58 (62%)	36 (100%)	0	100	100
3	R	261/539 (48%)	260 (100%)	1 (0%)	84	84
4	A	180/305 (59%)	180 (100%)	0	100	100
All	All	745/1203 (62%)	744 (100%)	1 (0%)	87	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	R	179	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 9 such sidechains are listed below:

Mol	Chain	Res	Type
4	A	52	GLN
4	A	322	HIS
3	R	185	ASN
3	R	190	ASN
3	R	225	HIS

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)

4 ligands 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	$\#\|Z\| > 2$
5	CLR	R	503	-	31,31,31	0.38	0	48,48,48	0.82	0
5	CLR	R	501	-	31,31,31	0.40	0	48,48,48	0.61	0
5	CLR	R	502	-	31,31,31	0.38	0	48,48,48	0.78	1 (2%)
6	A1BK1	R	504	-	50,50,50	0.94	3 (6%)	69,77,77	0.99	4 (5%)

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
5	CLR	R	503	-	-	4/10/68/68	0/4/4/4
5	CLR	R	501	-	-	1/10/68/68	0/4/4/4
5	CLR	R	502	-	-	1/10/68/68	0/4/4/4
6	A1BK1	R	504	-	-	11/21/78/78	0/9/8/8

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	R	504	A1BK1	C22-N2	3.97	1.41	1.35
6	R	504	A1BK1	C18-C19	2.09	1.56	1.53
6	R	504	A1BK1	C16-C12	-2.02	1.35	1.38

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	R	504	A1BK1	O1-C2-C1	-2.27	103.26	107.97
6	R	504	A1BK1	C18-C19-N2	2.20	115.12	112.69
6	R	504	A1BK1	C16-O3-C18	-2.12	101.76	106.18
5	R	502	CLR	C13-C17-C20	2.10	122.73	119.50
6	R	504	A1BK1	C1-C2-C3	2.01	115.91	113.81

There are no chirality outliers.

5 of 17 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	R	504	A1BK1	C20-C19-N2-C21
6	R	504	A1BK1	C27-C28-N3-N4
6	R	504	A1BK1	C31-C30-N4-N3
6	R	504	A1BK1	C29-C28-N3-N4
6	R	504	A1BK1	C32-C30-N4-N3

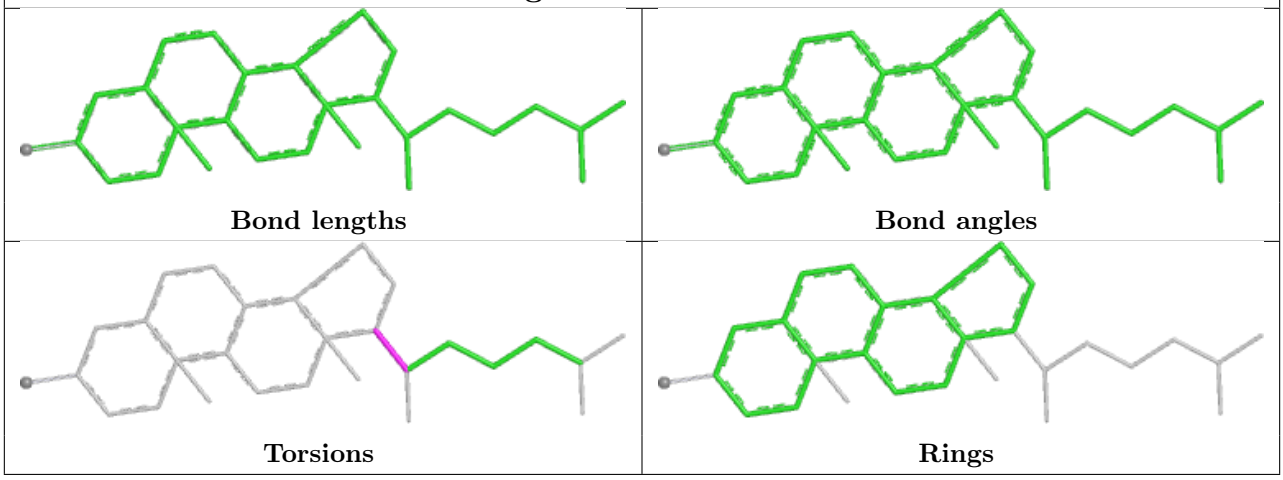
There are no ring outliers.

2 monomers are involved in 2 short contacts:

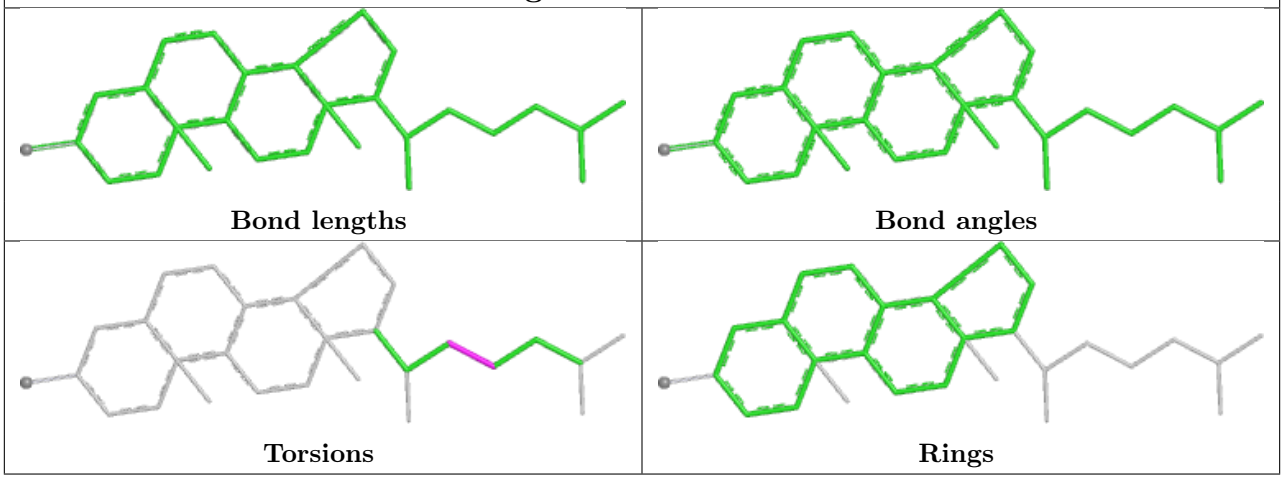
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	R	503	CLR	1	0
5	R	501	CLR	1	0

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.

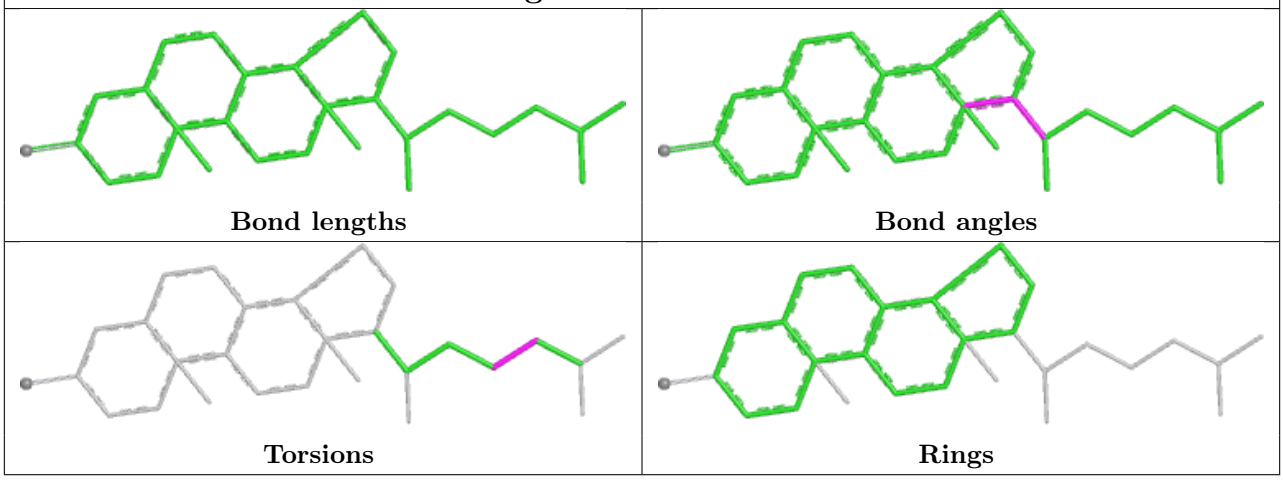
Ligand CLR R 503



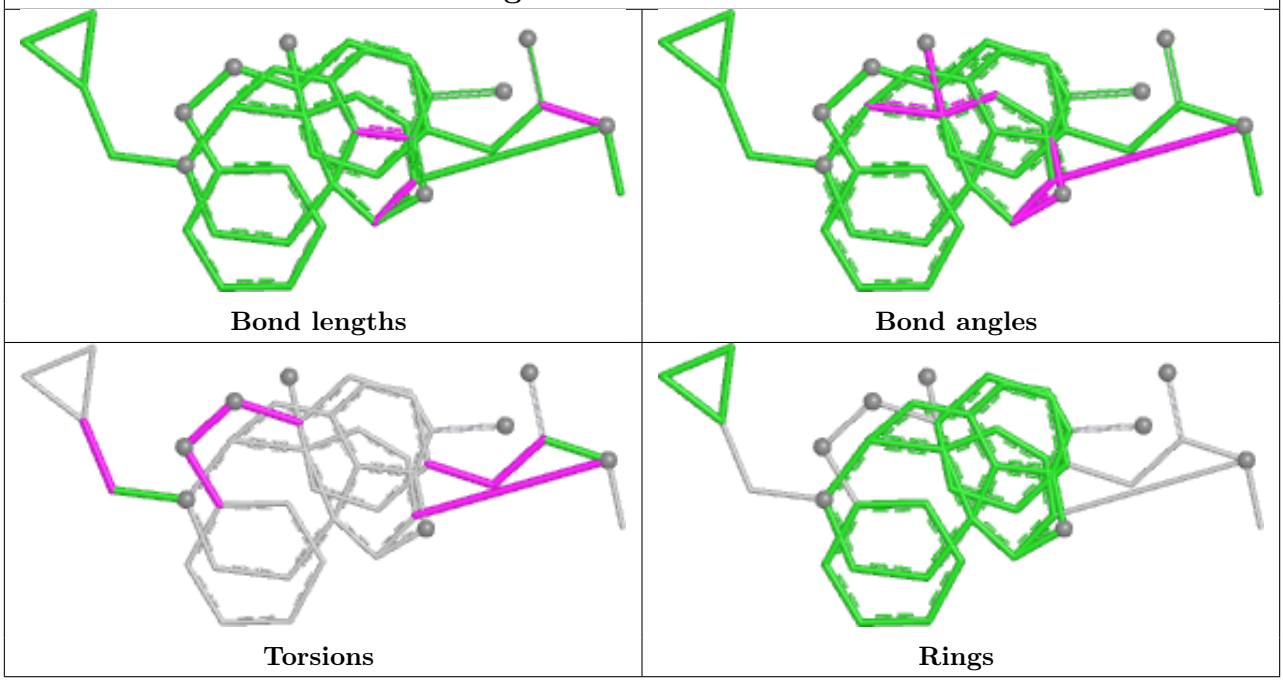
Ligand CLR R 501



Ligand CLR R 502



Ligand A1BK1 R 504



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.

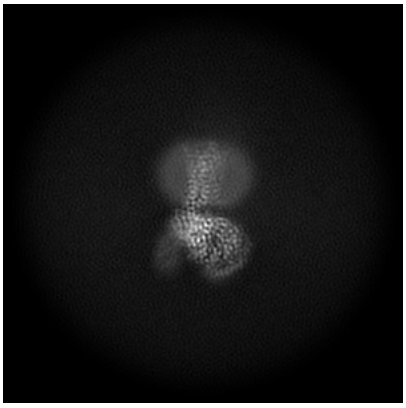
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-72952. These allow visual inspection of the internal detail of the map and identification of artifacts.

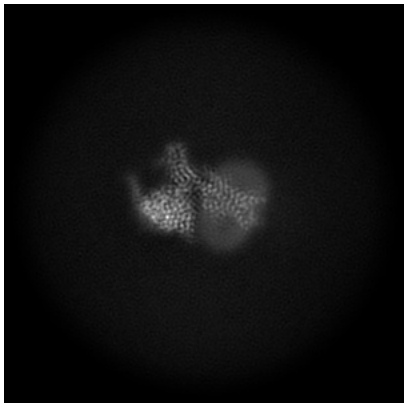
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

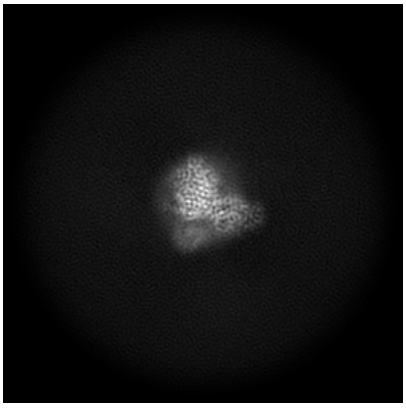
6.1.1 Primary map



X



Y



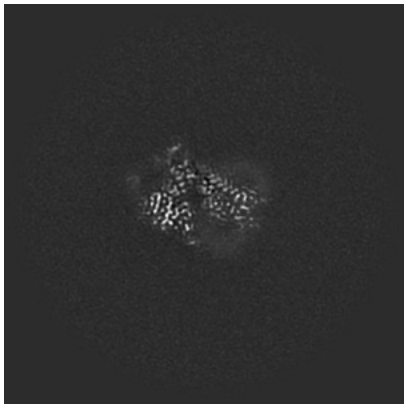
Z

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

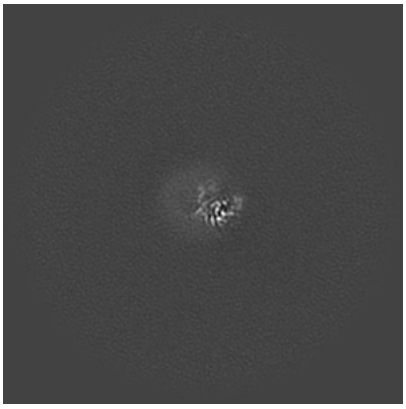
6.2 Central slices (i)

6.2.1 Primary map

X Index: 128



Y Index: 128

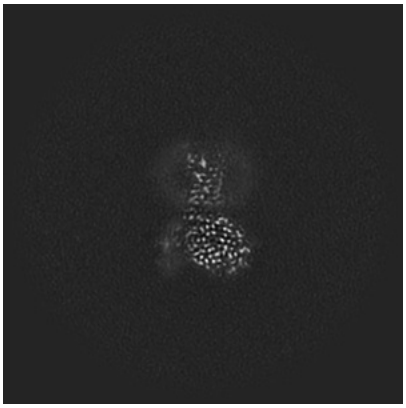


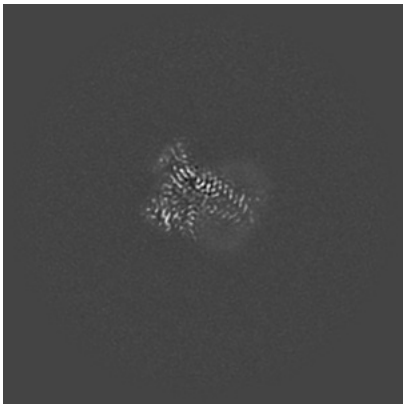
Z Index: 128

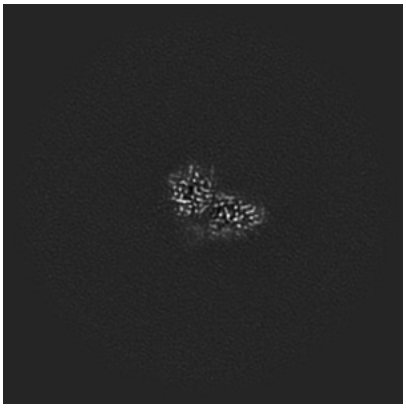
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 125

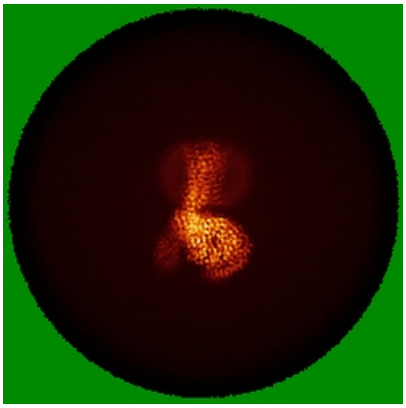

Y Index: 121

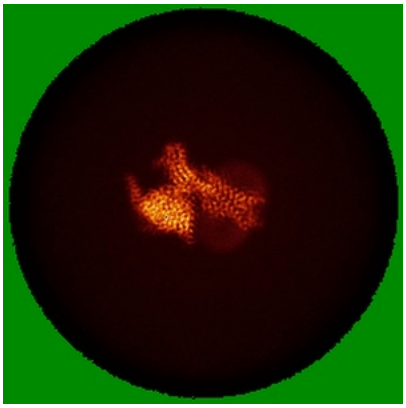

Z Index: 113

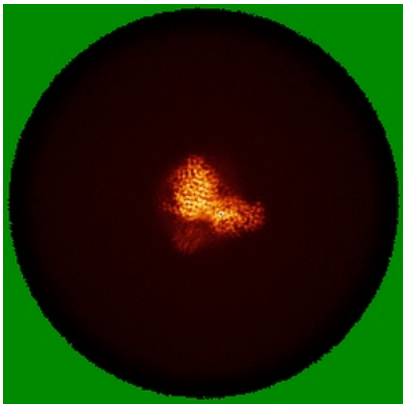
The images above show the largest variance slices of the map in three orthogonal directions.

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

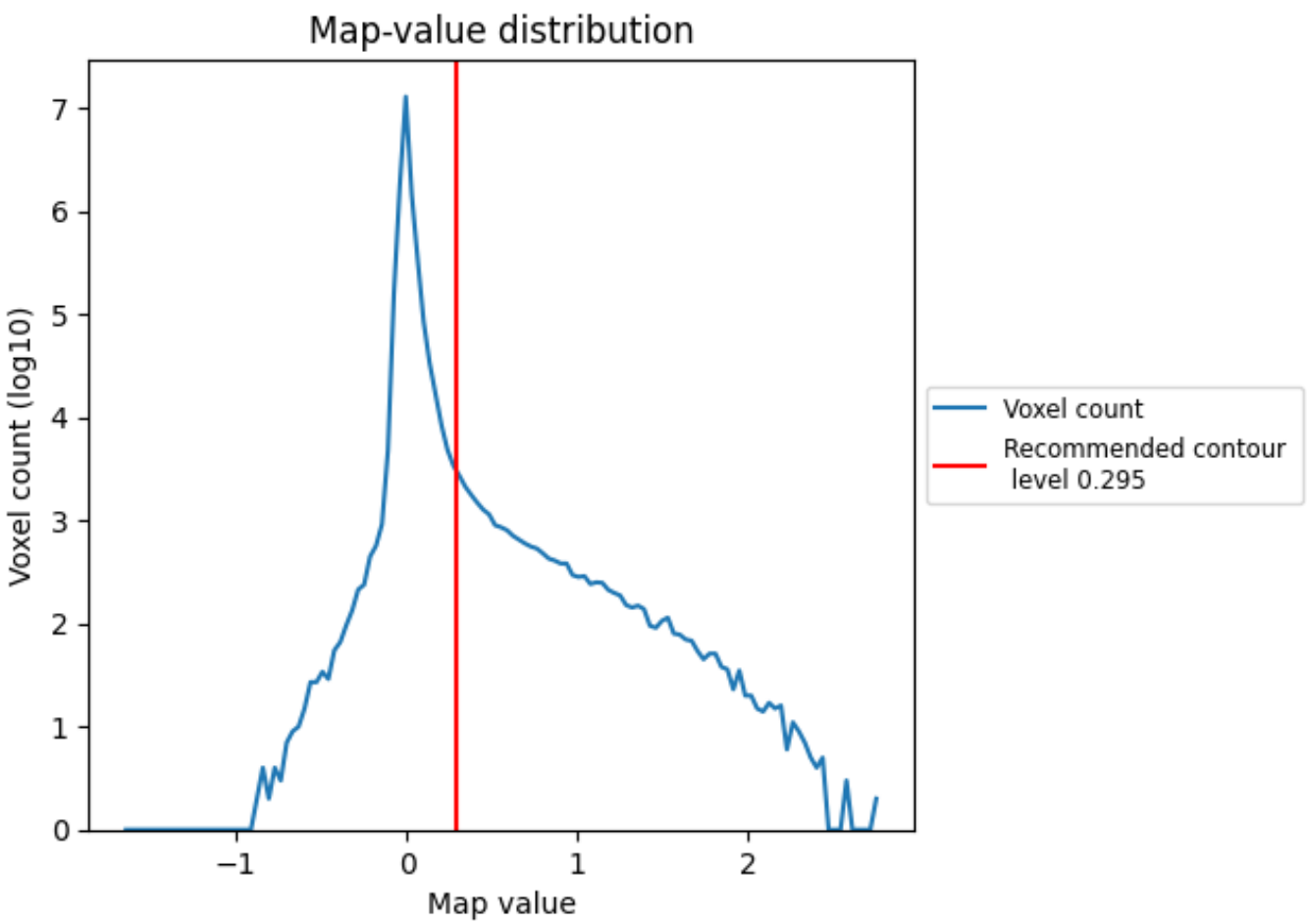
6.6 Mask visualisation (i)

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

7 Map analysis (i)

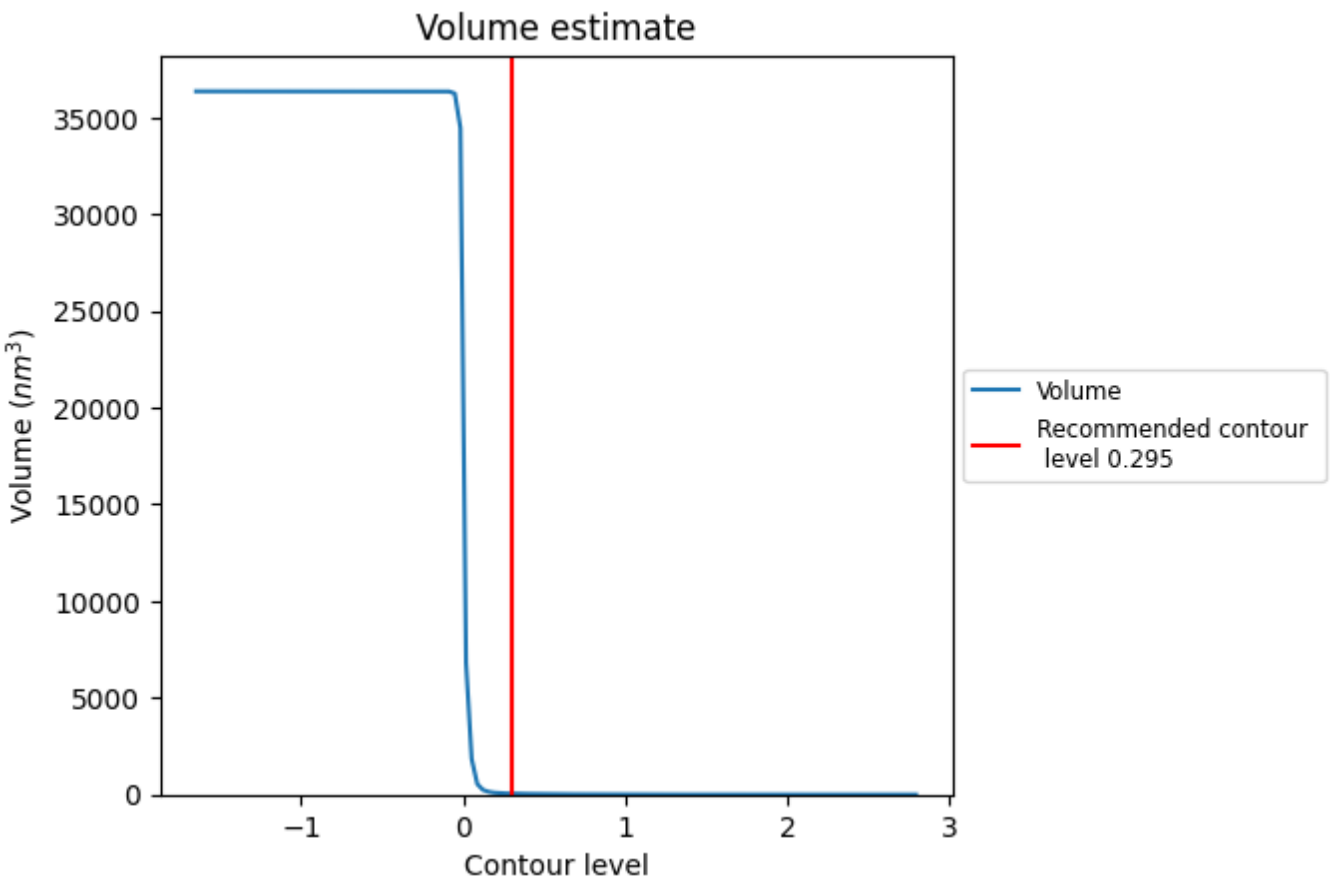
This section contains the results of statistical analysis of the map.

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.

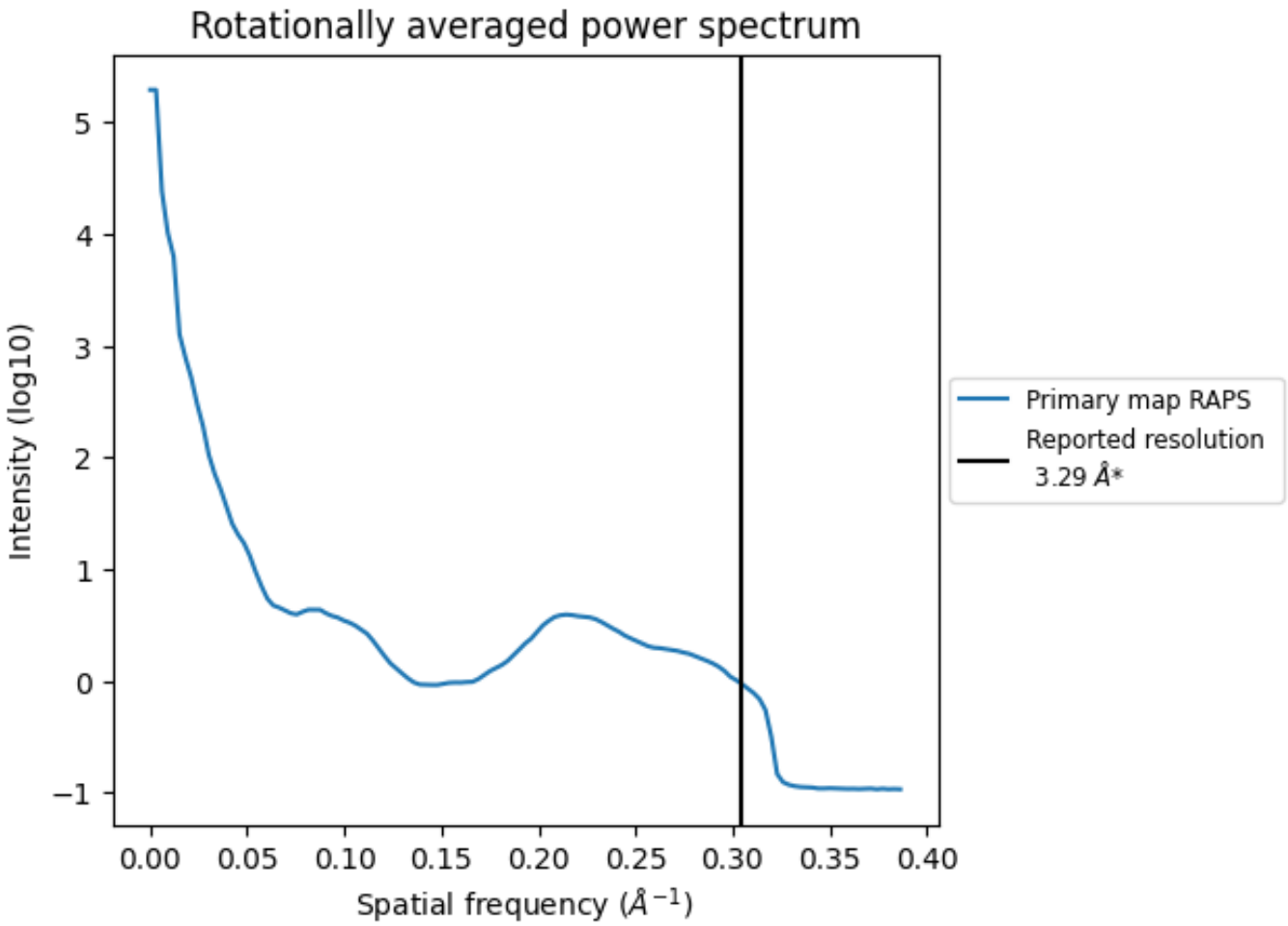
7.2 Volume estimate (i)



The volume at the recommended contour level is 51 nm^3; this corresponds to an approximate mass of 46 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 0.304 Å^{-1}

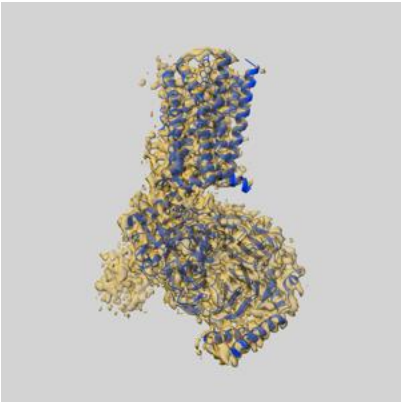
8 Fourier-Shell correlation (i)

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

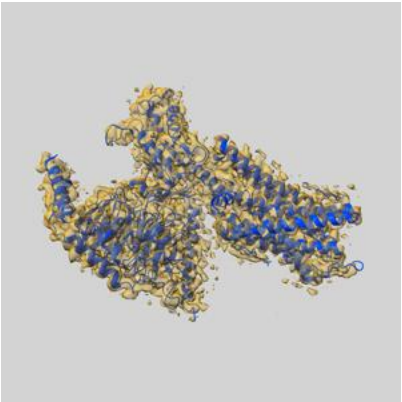
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-72952 and PDB model 9YH3. Per-residue inclusion information can be found in section 3 on page 12.

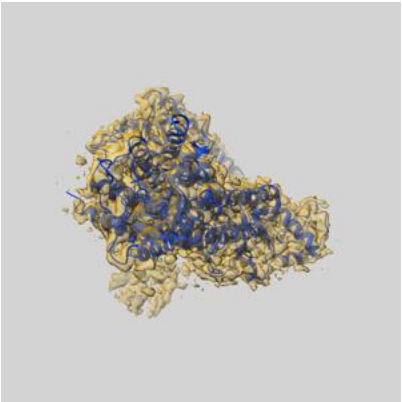
9.1 Map-model overlay (i)



X



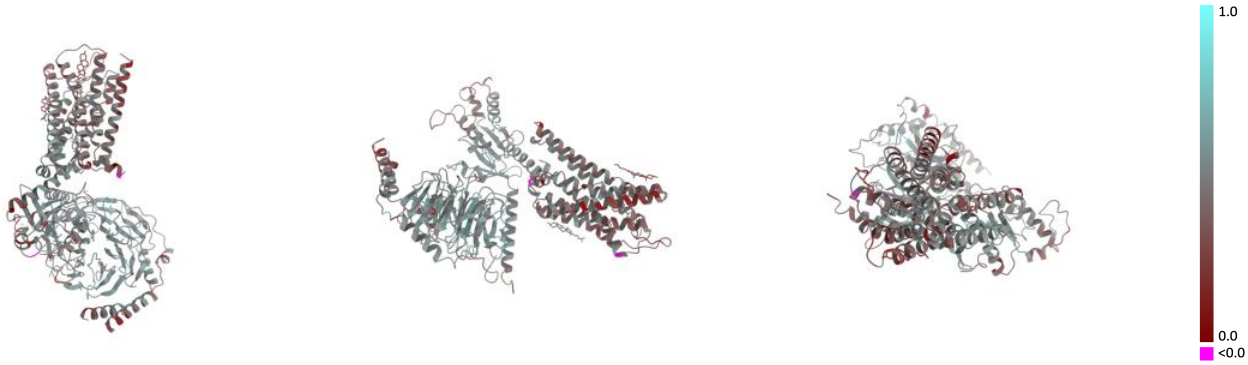
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.295 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.

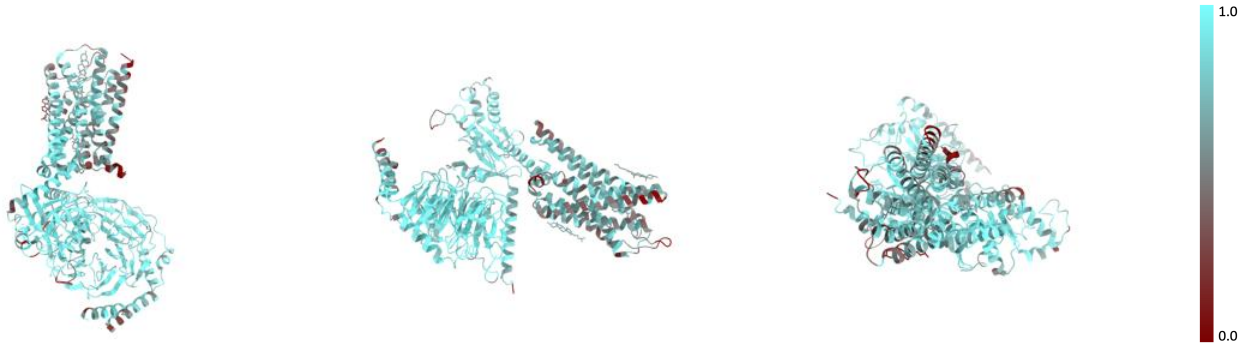
9.2 Q-score mapped to coordinate model (i)



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.

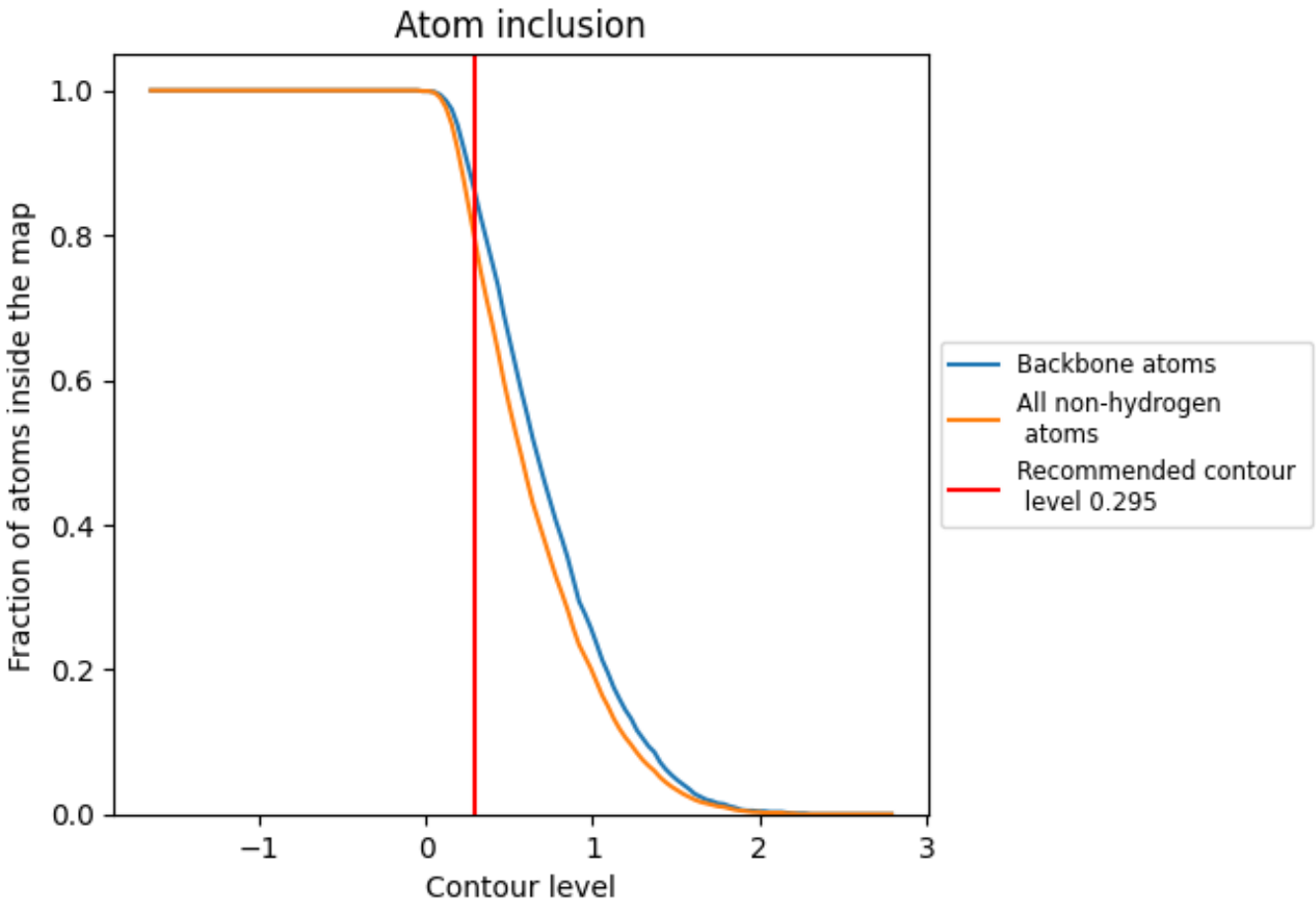
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.295).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 79% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.295) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7930	0.4660
A	0.8280	0.4750
B	0.8860	0.5220
C	0.8250	0.4740
R	0.6660	0.3990