



Full wwPDB EM Validation Report ⓘ

Aug 5, 2026 – 03:23 AM EDT

PDB ID : 8DHB / pdb_00008dhb
EMDB ID : EMD-27435
Title : Active FLCN GAP complex
Authors : Jansen, R.M.; Hurley, J.H.
Deposited on : 2022-06-25
Resolution : 3.53 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:

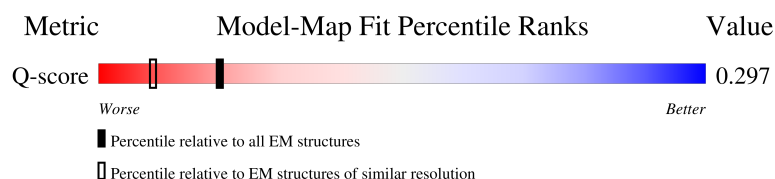
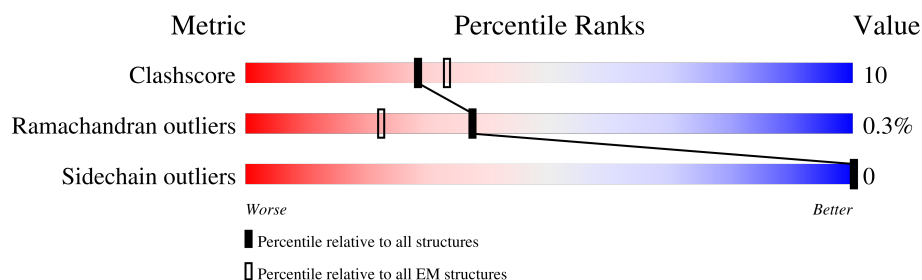
EMDB validation analysis : 0.0.1.dev133
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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) : 2.50

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 3.53 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	12947 (3.03 - 4.02)

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	400	8% 54% 22% 24%
2	B	336	35% 61% 21% 18%
3	C	166	37% 47% 8% 45%
4	D	127	23% 70% 24% 6%

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Mol	Chain	Length	Quality of chain
5	E	124	
6	F	99	
7	G	173	
8	H	356	
9	I	1351	
10	J	622	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	CZC	A	501	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 15171 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 Ras-related GTP-binding protein C.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	306	Total	C	N	O	S	0	0
			2486	1604	400	468	14		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	181	ASN	ASP	conflict	UNP Q9HB90
A	400	LEU	-	expression tag	UNP Q9HB90

- Molecule 2 is a protein called Ras-related GTP-binding protein A.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	277	Total	C	N	O	S	0	0
			2291	1463	392	419	17		

There are 23 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-22	MET	-	expression tag	UNP Q7L523
B	-21	SER	-	expression tag	UNP Q7L523
B	-20	TRP	-	expression tag	UNP Q7L523
B	-19	SER	-	expression tag	UNP Q7L523
B	-18	HIS	-	expression tag	UNP Q7L523
B	-17	PRO	-	expression tag	UNP Q7L523
B	-16	GLN	-	expression tag	UNP Q7L523
B	-15	PHE	-	expression tag	UNP Q7L523
B	-14	GLU	-	expression tag	UNP Q7L523
B	-13	LYS	-	expression tag	UNP Q7L523
B	-12	GLY	-	expression tag	UNP Q7L523
B	-11	GLY	-	expression tag	UNP Q7L523
B	-10	PHE	-	expression tag	UNP Q7L523
B	-9	ASP	-	expression tag	UNP Q7L523
B	-8	ILE	-	expression tag	UNP Q7L523

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	ASP	-	expression tag	UNP Q7L523
B	-6	TYR	-	expression tag	UNP Q7L523
B	-5	LYS	-	expression tag	UNP Q7L523
B	-4	ASP	-	expression tag	UNP Q7L523
B	-3	ASP	-	expression tag	UNP Q7L523
B	-2	ASP	-	expression tag	UNP Q7L523
B	-1	ASP	-	expression tag	UNP Q7L523
B	0	LYS	-	expression tag	UNP Q7L523

- Molecule 3 is a protein called Regulator complex protein LAMTOR1.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	92	Total	C	N	O	0	0
			717	457	122	138		

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-4	SER	-	expression tag	UNP Q6IAA8
C	-3	ASN	-	expression tag	UNP Q6IAA8
C	-2	ALA	-	expression tag	UNP Q6IAA8
C	-1	GLU	-	expression tag	UNP Q6IAA8
C	0	PHE	-	expression tag	UNP Q6IAA8
C	2	ALA	GLY	engineered mutation	UNP Q6IAA8

- Molecule 4 is a protein called Regulator complex protein LAMTOR2.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	120	Total	C	N	O	S	0	0
			905	569	155	174	7		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	GLY	-	expression tag	UNP Q9Y2Q5
D	0	ALA	-	expression tag	UNP Q9Y2Q5

- Molecule 5 is a protein called Regulator complex protein LAMTOR3.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	116	Total	C	N	O	S	0	0
			901	582	153	165	1		

- Molecule 6 is a protein called Regulator complex protein LAMTOR4.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	91	Total	C	N	O	S	0	0
			696	433	129	132	2		

- Molecule 7 is a protein called Regulator complex protein LAMTOR5.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	89	Total	C	N	O	S	0	0
			649	397	113	132	7		

- Molecule 8 is a protein called Glutathione S-transferase class-mu 26 kDa isozyme,Sodium-coupled neutral amino acid transporter 9 chimera.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	59	Total	C	N	O	S	0	0
			466	295	83	85	3		

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	-236	MET	-	initiating methionine	UNP P08515
H	-235	ALA	-	expression tag	UNP P08515
H	-17	SER	-	linker	UNP P08515
H	-16	ASP	-	linker	UNP P08515
H	-15	ASP	-	linker	UNP P08515
H	-14	TYR	-	linker	UNP P08515
H	-13	ASP	-	linker	UNP P08515
H	-12	ILE	-	linker	UNP P08515
H	-11	PRO	-	linker	UNP P08515
H	-10	THR	-	linker	UNP P08515
H	-9	THR	-	linker	UNP P08515
H	-8	GLU	-	linker	UNP P08515
H	-7	ASN	-	linker	UNP P08515
H	-6	LEU	-	linker	UNP P08515
H	-5	TYR	-	linker	UNP P08515
H	-4	PHE	-	linker	UNP P08515
H	-3	GLN	-	linker	UNP P08515
H	-2	GLY	-	linker	UNP P08515

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-1	GLY	-	linker	UNP P08515
H	0	THR	-	linker	UNP P08515

- Molecule 9 is a protein called Folliculin-interacting protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	387	Total	C	N	O	S	0	0
			3115	2012	528	553	22		

There are 237 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
I	-236	MET	-	initiating methionine	UNP Q9P278
I	-235	ALA	-	expression tag	UNP Q9P278
I	-234	SER	-	expression tag	UNP Q9P278
I	-233	PRO	-	expression tag	UNP Q9P278
I	-232	ILE	-	expression tag	UNP Q9P278
I	-231	LEU	-	expression tag	UNP Q9P278
I	-230	GLY	-	expression tag	UNP Q9P278
I	-229	TYR	-	expression tag	UNP Q9P278
I	-228	TRP	-	expression tag	UNP Q9P278
I	-227	LYS	-	expression tag	UNP Q9P278
I	-226	ILE	-	expression tag	UNP Q9P278
I	-225	LYS	-	expression tag	UNP Q9P278
I	-224	GLY	-	expression tag	UNP Q9P278
I	-223	LEU	-	expression tag	UNP Q9P278
I	-222	VAL	-	expression tag	UNP Q9P278
I	-221	GLN	-	expression tag	UNP Q9P278
I	-220	PRO	-	expression tag	UNP Q9P278
I	-219	THR	-	expression tag	UNP Q9P278
I	-218	ARG	-	expression tag	UNP Q9P278
I	-217	LEU	-	expression tag	UNP Q9P278
I	-216	LEU	-	expression tag	UNP Q9P278
I	-215	LEU	-	expression tag	UNP Q9P278
I	-214	GLU	-	expression tag	UNP Q9P278
I	-213	TYR	-	expression tag	UNP Q9P278
I	-212	LEU	-	expression tag	UNP Q9P278
I	-211	GLU	-	expression tag	UNP Q9P278
I	-210	GLU	-	expression tag	UNP Q9P278
I	-209	LYS	-	expression tag	UNP Q9P278
I	-208	TYR	-	expression tag	UNP Q9P278
I	-207	GLU	-	expression tag	UNP Q9P278

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-206	GLU	-	expression tag	UNP Q9P278
I	-205	HIS	-	expression tag	UNP Q9P278
I	-204	LEU	-	expression tag	UNP Q9P278
I	-203	TYR	-	expression tag	UNP Q9P278
I	-202	GLU	-	expression tag	UNP Q9P278
I	-201	ARG	-	expression tag	UNP Q9P278
I	-200	ASP	-	expression tag	UNP Q9P278
I	-199	GLU	-	expression tag	UNP Q9P278
I	-198	GLY	-	expression tag	UNP Q9P278
I	-197	ASP	-	expression tag	UNP Q9P278
I	-196	LYS	-	expression tag	UNP Q9P278
I	-195	TRP	-	expression tag	UNP Q9P278
I	-194	ARG	-	expression tag	UNP Q9P278
I	-193	ASN	-	expression tag	UNP Q9P278
I	-192	LYS	-	expression tag	UNP Q9P278
I	-191	LYS	-	expression tag	UNP Q9P278
I	-190	PHE	-	expression tag	UNP Q9P278
I	-189	GLU	-	expression tag	UNP Q9P278
I	-188	LEU	-	expression tag	UNP Q9P278
I	-187	GLY	-	expression tag	UNP Q9P278
I	-186	LEU	-	expression tag	UNP Q9P278
I	-185	GLU	-	expression tag	UNP Q9P278
I	-184	PHE	-	expression tag	UNP Q9P278
I	-183	PRO	-	expression tag	UNP Q9P278
I	-182	ASN	-	expression tag	UNP Q9P278
I	-181	LEU	-	expression tag	UNP Q9P278
I	-180	PRO	-	expression tag	UNP Q9P278
I	-179	TYR	-	expression tag	UNP Q9P278
I	-178	TYR	-	expression tag	UNP Q9P278
I	-177	ILE	-	expression tag	UNP Q9P278
I	-176	ASP	-	expression tag	UNP Q9P278
I	-175	GLY	-	expression tag	UNP Q9P278
I	-174	ASP	-	expression tag	UNP Q9P278
I	-173	VAL	-	expression tag	UNP Q9P278
I	-172	LYS	-	expression tag	UNP Q9P278
I	-171	LEU	-	expression tag	UNP Q9P278
I	-170	THR	-	expression tag	UNP Q9P278
I	-169	GLN	-	expression tag	UNP Q9P278
I	-168	SER	-	expression tag	UNP Q9P278
I	-167	MET	-	expression tag	UNP Q9P278
I	-166	ALA	-	expression tag	UNP Q9P278
I	-165	ILE	-	expression tag	UNP Q9P278

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-164	ILE	-	expression tag	UNP Q9P278
I	-163	ARG	-	expression tag	UNP Q9P278
I	-162	TYR	-	expression tag	UNP Q9P278
I	-161	ILE	-	expression tag	UNP Q9P278
I	-160	ALA	-	expression tag	UNP Q9P278
I	-159	ASP	-	expression tag	UNP Q9P278
I	-158	LYS	-	expression tag	UNP Q9P278
I	-157	HIS	-	expression tag	UNP Q9P278
I	-156	ASN	-	expression tag	UNP Q9P278
I	-155	MET	-	expression tag	UNP Q9P278
I	-154	LEU	-	expression tag	UNP Q9P278
I	-153	GLY	-	expression tag	UNP Q9P278
I	-152	GLY	-	expression tag	UNP Q9P278
I	-151	CYS	-	expression tag	UNP Q9P278
I	-150	PRO	-	expression tag	UNP Q9P278
I	-149	LYS	-	expression tag	UNP Q9P278
I	-148	GLU	-	expression tag	UNP Q9P278
I	-147	ARG	-	expression tag	UNP Q9P278
I	-146	ALA	-	expression tag	UNP Q9P278
I	-145	GLU	-	expression tag	UNP Q9P278
I	-144	ILE	-	expression tag	UNP Q9P278
I	-143	SER	-	expression tag	UNP Q9P278
I	-142	MET	-	expression tag	UNP Q9P278
I	-141	LEU	-	expression tag	UNP Q9P278
I	-140	GLU	-	expression tag	UNP Q9P278
I	-139	GLY	-	expression tag	UNP Q9P278
I	-138	ALA	-	expression tag	UNP Q9P278
I	-137	VAL	-	expression tag	UNP Q9P278
I	-136	LEU	-	expression tag	UNP Q9P278
I	-135	ASP	-	expression tag	UNP Q9P278
I	-134	ILE	-	expression tag	UNP Q9P278
I	-133	ARG	-	expression tag	UNP Q9P278
I	-132	TYR	-	expression tag	UNP Q9P278
I	-131	GLY	-	expression tag	UNP Q9P278
I	-130	VAL	-	expression tag	UNP Q9P278
I	-129	SER	-	expression tag	UNP Q9P278
I	-128	ARG	-	expression tag	UNP Q9P278
I	-127	ILE	-	expression tag	UNP Q9P278
I	-126	ALA	-	expression tag	UNP Q9P278
I	-125	TYR	-	expression tag	UNP Q9P278
I	-124	SER	-	expression tag	UNP Q9P278
I	-123	LYS	-	expression tag	UNP Q9P278

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-122	ASP	-	expression tag	UNP Q9P278
I	-121	PHE	-	expression tag	UNP Q9P278
I	-120	GLU	-	expression tag	UNP Q9P278
I	-119	THR	-	expression tag	UNP Q9P278
I	-118	LEU	-	expression tag	UNP Q9P278
I	-117	LYS	-	expression tag	UNP Q9P278
I	-116	VAL	-	expression tag	UNP Q9P278
I	-115	ASP	-	expression tag	UNP Q9P278
I	-114	PHE	-	expression tag	UNP Q9P278
I	-113	LEU	-	expression tag	UNP Q9P278
I	-112	SER	-	expression tag	UNP Q9P278
I	-111	LYS	-	expression tag	UNP Q9P278
I	-110	LEU	-	expression tag	UNP Q9P278
I	-109	PRO	-	expression tag	UNP Q9P278
I	-108	GLU	-	expression tag	UNP Q9P278
I	-107	MET	-	expression tag	UNP Q9P278
I	-106	LEU	-	expression tag	UNP Q9P278
I	-105	LYS	-	expression tag	UNP Q9P278
I	-104	MET	-	expression tag	UNP Q9P278
I	-103	PHE	-	expression tag	UNP Q9P278
I	-102	GLU	-	expression tag	UNP Q9P278
I	-101	ASP	-	expression tag	UNP Q9P278
I	-100	ARG	-	expression tag	UNP Q9P278
I	-99	LEU	-	expression tag	UNP Q9P278
I	-98	CYS	-	expression tag	UNP Q9P278
I	-97	HIS	-	expression tag	UNP Q9P278
I	-96	LYS	-	expression tag	UNP Q9P278
I	-95	THR	-	expression tag	UNP Q9P278
I	-94	TYR	-	expression tag	UNP Q9P278
I	-93	LEU	-	expression tag	UNP Q9P278
I	-92	ASN	-	expression tag	UNP Q9P278
I	-91	GLY	-	expression tag	UNP Q9P278
I	-90	ASP	-	expression tag	UNP Q9P278
I	-89	HIS	-	expression tag	UNP Q9P278
I	-88	VAL	-	expression tag	UNP Q9P278
I	-87	THR	-	expression tag	UNP Q9P278
I	-86	HIS	-	expression tag	UNP Q9P278
I	-85	PRO	-	expression tag	UNP Q9P278
I	-84	ASP	-	expression tag	UNP Q9P278
I	-83	PHE	-	expression tag	UNP Q9P278
I	-82	MET	-	expression tag	UNP Q9P278
I	-81	LEU	-	expression tag	UNP Q9P278

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-80	TYR	-	expression tag	UNP Q9P278
I	-79	ASP	-	expression tag	UNP Q9P278
I	-78	ALA	-	expression tag	UNP Q9P278
I	-77	LEU	-	expression tag	UNP Q9P278
I	-76	ASP	-	expression tag	UNP Q9P278
I	-75	VAL	-	expression tag	UNP Q9P278
I	-74	VAL	-	expression tag	UNP Q9P278
I	-73	LEU	-	expression tag	UNP Q9P278
I	-72	TYR	-	expression tag	UNP Q9P278
I	-71	MET	-	expression tag	UNP Q9P278
I	-70	ASP	-	expression tag	UNP Q9P278
I	-69	PRO	-	expression tag	UNP Q9P278
I	-68	MET	-	expression tag	UNP Q9P278
I	-67	CYS	-	expression tag	UNP Q9P278
I	-66	LEU	-	expression tag	UNP Q9P278
I	-65	ASP	-	expression tag	UNP Q9P278
I	-64	ALA	-	expression tag	UNP Q9P278
I	-63	PHE	-	expression tag	UNP Q9P278
I	-62	PRO	-	expression tag	UNP Q9P278
I	-61	LYS	-	expression tag	UNP Q9P278
I	-60	LEU	-	expression tag	UNP Q9P278
I	-59	VAL	-	expression tag	UNP Q9P278
I	-58	CYS	-	expression tag	UNP Q9P278
I	-57	PHE	-	expression tag	UNP Q9P278
I	-56	LYS	-	expression tag	UNP Q9P278
I	-55	LYS	-	expression tag	UNP Q9P278
I	-54	ARG	-	expression tag	UNP Q9P278
I	-53	ILE	-	expression tag	UNP Q9P278
I	-52	GLU	-	expression tag	UNP Q9P278
I	-51	ALA	-	expression tag	UNP Q9P278
I	-50	ILE	-	expression tag	UNP Q9P278
I	-49	PRO	-	expression tag	UNP Q9P278
I	-48	GLN	-	expression tag	UNP Q9P278
I	-47	ILE	-	expression tag	UNP Q9P278
I	-46	ASP	-	expression tag	UNP Q9P278
I	-45	LYS	-	expression tag	UNP Q9P278
I	-44	TYR	-	expression tag	UNP Q9P278
I	-43	LEU	-	expression tag	UNP Q9P278
I	-42	LYS	-	expression tag	UNP Q9P278
I	-41	SER	-	expression tag	UNP Q9P278
I	-40	SER	-	expression tag	UNP Q9P278
I	-39	LYS	-	expression tag	UNP Q9P278

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Chain	Residue	Modelled	Actual	Comment	Reference
I	-38	TYR	-	expression tag	UNP Q9P278
I	-37	ILE	-	expression tag	UNP Q9P278
I	-36	ALA	-	expression tag	UNP Q9P278
I	-35	TRP	-	expression tag	UNP Q9P278
I	-34	PRO	-	expression tag	UNP Q9P278
I	-33	LEU	-	expression tag	UNP Q9P278
I	-32	GLN	-	expression tag	UNP Q9P278
I	-31	GLY	-	expression tag	UNP Q9P278
I	-30	TRP	-	expression tag	UNP Q9P278
I	-29	GLN	-	expression tag	UNP Q9P278
I	-28	ALA	-	expression tag	UNP Q9P278
I	-27	THR	-	expression tag	UNP Q9P278
I	-26	PHE	-	expression tag	UNP Q9P278
I	-25	GLY	-	expression tag	UNP Q9P278
I	-24	GLY	-	expression tag	UNP Q9P278
I	-23	GLY	-	expression tag	UNP Q9P278
I	-22	ASP	-	expression tag	UNP Q9P278
I	-21	HIS	-	expression tag	UNP Q9P278
I	-20	PRO	-	expression tag	UNP Q9P278
I	-19	PRO	-	expression tag	UNP Q9P278
I	-18	LYS	-	expression tag	UNP Q9P278
I	-17	SER	-	expression tag	UNP Q9P278
I	-16	ASP	-	expression tag	UNP Q9P278
I	-15	ASP	-	expression tag	UNP Q9P278
I	-14	TYR	-	expression tag	UNP Q9P278
I	-13	ASP	-	expression tag	UNP Q9P278
I	-12	ILE	-	expression tag	UNP Q9P278
I	-11	PRO	-	expression tag	UNP Q9P278
I	-10	THR	-	expression tag	UNP Q9P278
I	-9	THR	-	expression tag	UNP Q9P278
I	-8	GLU	-	expression tag	UNP Q9P278
I	-7	ASN	-	expression tag	UNP Q9P278
I	-6	LEU	-	expression tag	UNP Q9P278
I	-5	TYR	-	expression tag	UNP Q9P278
I	-4	PHE	-	expression tag	UNP Q9P278
I	-3	GLN	-	expression tag	UNP Q9P278
I	-2	GLY	-	expression tag	UNP Q9P278
I	-1	GLY	-	expression tag	UNP Q9P278
I	0	THR	-	expression tag	UNP Q9P278

- Molecule 10 is a protein called Folliculin.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	361	Total	C	N	O	S	0	0
			2885	1865	494	506	20		

There are 43 discrepancies between the modelled and reference sequences:

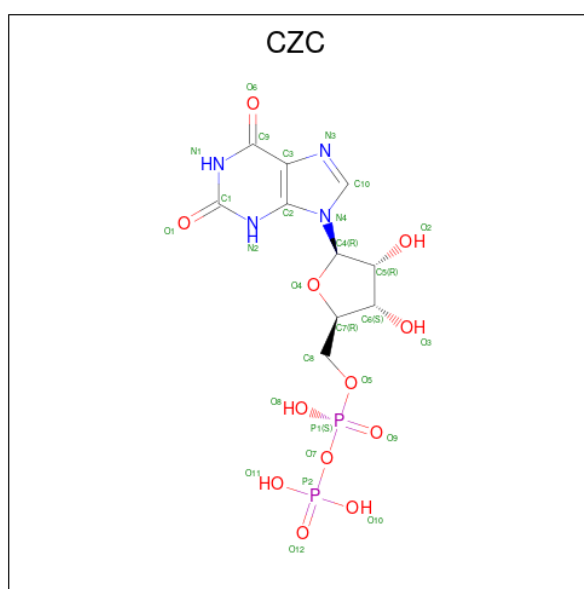
Chain	Residue	Modelled	Actual	Comment	Reference
J	-42	MET	-	initiating methionine	UNP Q8NFG4
J	-41	ALA	-	expression tag	UNP Q8NFG4
J	-40	SER	-	expression tag	UNP Q8NFG4
J	-39	TRP	-	expression tag	UNP Q8NFG4
J	-38	SER	-	expression tag	UNP Q8NFG4
J	-37	HIS	-	expression tag	UNP Q8NFG4
J	-36	PRO	-	expression tag	UNP Q8NFG4
J	-35	GLN	-	expression tag	UNP Q8NFG4
J	-34	PHE	-	expression tag	UNP Q8NFG4
J	-33	GLU	-	expression tag	UNP Q8NFG4
J	-32	LYS	-	expression tag	UNP Q8NFG4
J	-31	GLY	-	expression tag	UNP Q8NFG4
J	-30	GLY	-	expression tag	UNP Q8NFG4
J	-29	GLY	-	expression tag	UNP Q8NFG4
J	-28	ALA	-	expression tag	UNP Q8NFG4
J	-27	ARG	-	expression tag	UNP Q8NFG4
J	-26	GLY	-	expression tag	UNP Q8NFG4
J	-25	GLY	-	expression tag	UNP Q8NFG4
J	-24	SER	-	expression tag	UNP Q8NFG4
J	-23	GLY	-	expression tag	UNP Q8NFG4
J	-22	GLY	-	expression tag	UNP Q8NFG4
J	-21	GLY	-	expression tag	UNP Q8NFG4
J	-20	SER	-	expression tag	UNP Q8NFG4
J	-19	TRP	-	expression tag	UNP Q8NFG4
J	-18	SER	-	expression tag	UNP Q8NFG4
J	-17	HIS	-	expression tag	UNP Q8NFG4
J	-16	PRO	-	expression tag	UNP Q8NFG4
J	-15	GLN	-	expression tag	UNP Q8NFG4
J	-14	PHE	-	expression tag	UNP Q8NFG4
J	-13	GLU	-	expression tag	UNP Q8NFG4
J	-12	LYS	-	expression tag	UNP Q8NFG4
J	-11	GLY	-	expression tag	UNP Q8NFG4
J	-10	PHE	-	expression tag	UNP Q8NFG4
J	-9	ASP	-	expression tag	UNP Q8NFG4
J	-8	TYR	-	expression tag	UNP Q8NFG4
J	-7	LYS	-	expression tag	UNP Q8NFG4
J	-6	ASP	-	expression tag	UNP Q8NFG4

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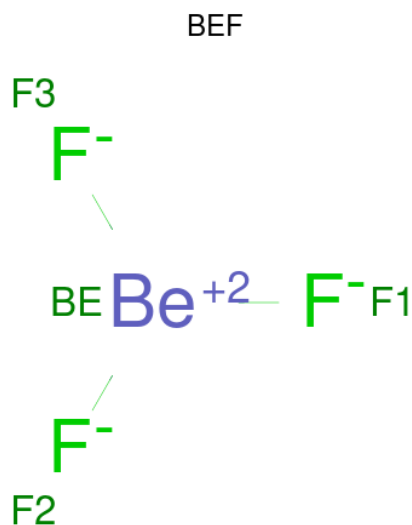
Chain	Residue	Modelled	Actual	Comment	Reference
J	-5	ASP	-	expression tag	UNP Q8NFG4
J	-4	ASP	-	expression tag	UNP Q8NFG4
J	-3	ASP	-	expression tag	UNP Q8NFG4
J	-2	LYS	-	expression tag	UNP Q8NFG4
J	-1	GLY	-	expression tag	UNP Q8NFG4
J	0	THR	-	expression tag	UNP Q8NFG4

- Molecule 11 is [(2 {R},3 {S},4 {R},5 {R})-5-[2,6-bis(oxidanylidene)-3 {H}-purin-9-yl]-3,4-bis(oxidanyl)oxolan-2-yl]methyl phosphono hydrogen phosphate (CCD ID: CZC) (formula: C₁₀H₁₄N₄O₁₂P₂) (labeled as "Ligand of Interest" by depositor).



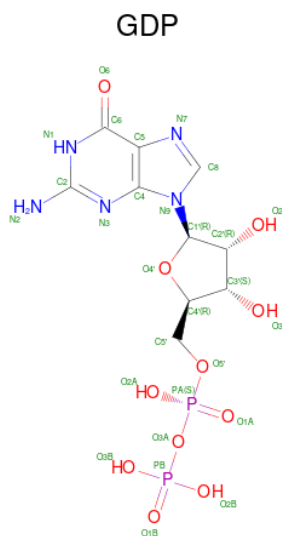
Mol	Chain	Residues	Atoms					AltConf
11	A	1	Total	C	N	O	P	0
			28	10	4	12	2	

- Molecule 12 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃) (labeled as "Ligand of Interest" by depositor).

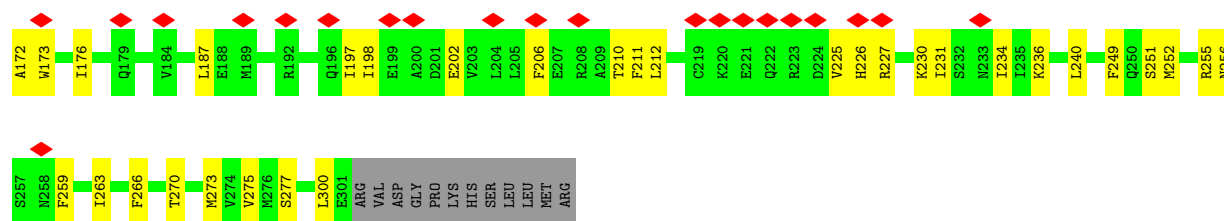


Mol	Chain	Residues	Atoms			AltConf
12	A	1	Total 4	Be 1	F 3	0

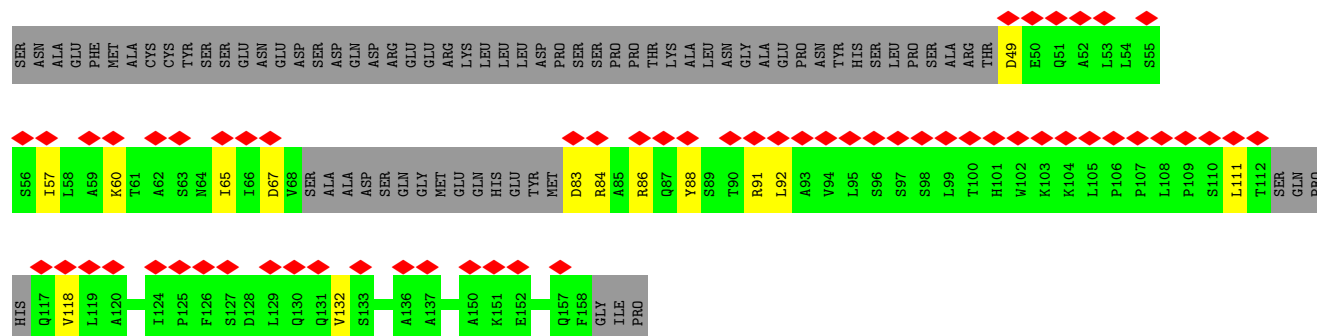
- Molecule 13 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



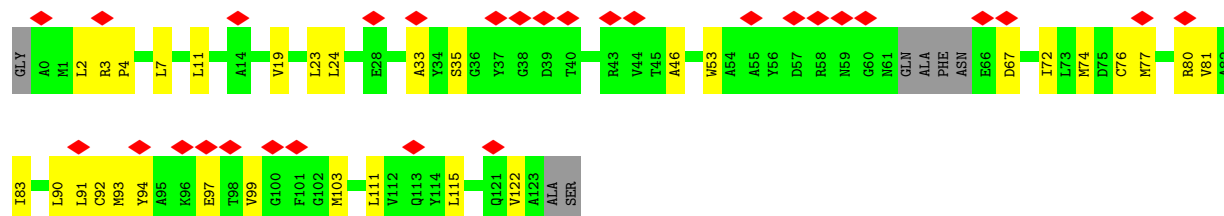
Mol	Chain	Residues	Atoms					AltConf
13	B	1	Total 28	C 10	N 5	O 11	P 2	0



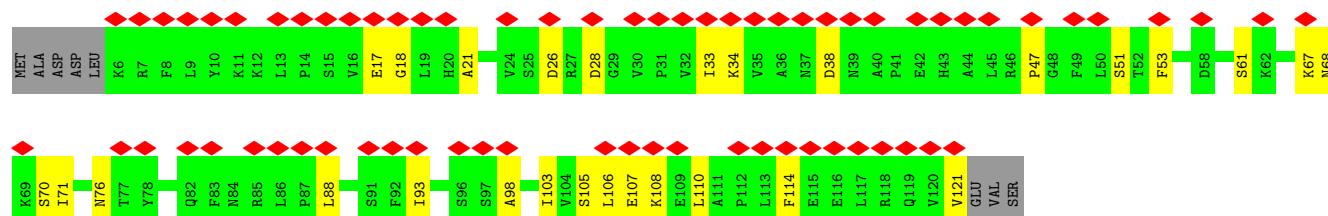
• Molecule 3: Ragulator complex protein LAMTOR1



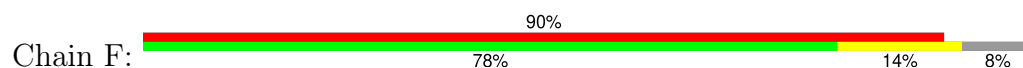
• Molecule 4: Ragulator complex protein LAMTOR2

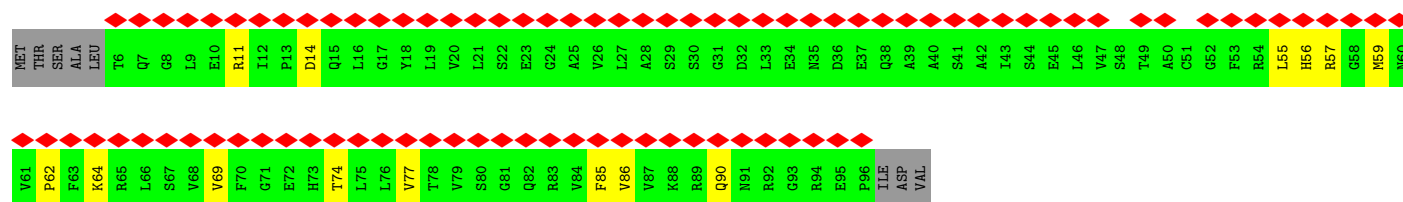


• Molecule 5: Ragulator complex protein LAMTOR3

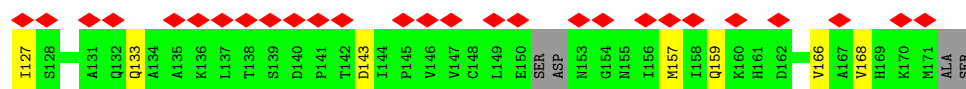


• Molecule 6: Ragulator complex protein LAMTOR4

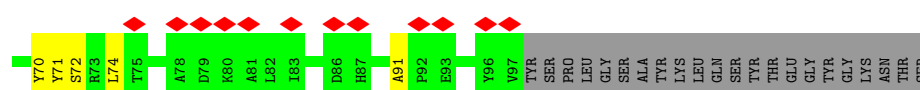
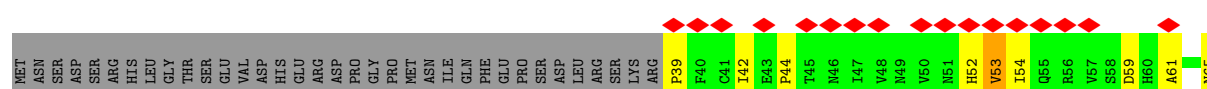
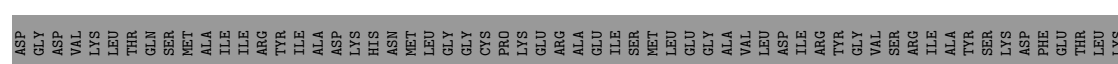
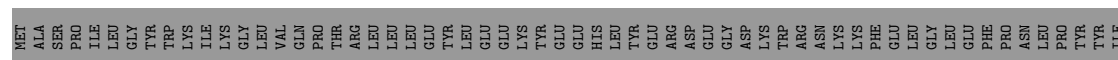




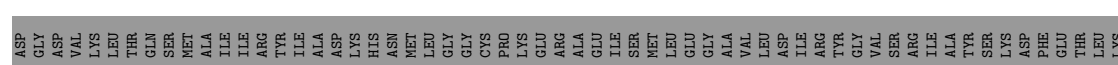
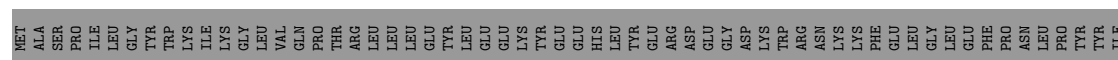
• Molecule 7: Ragulator complex protein LAMTOR5



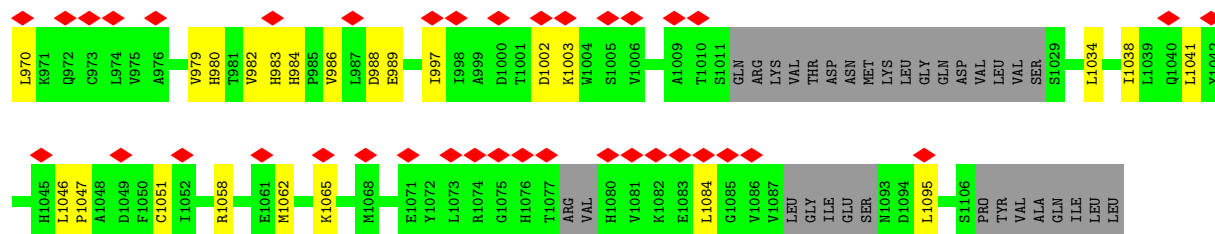
• Molecule 8: Glutathione S-transferase class-mu 26 kDa isozyme, Sodium-coupled neutral amino acid transporter 9 chimera



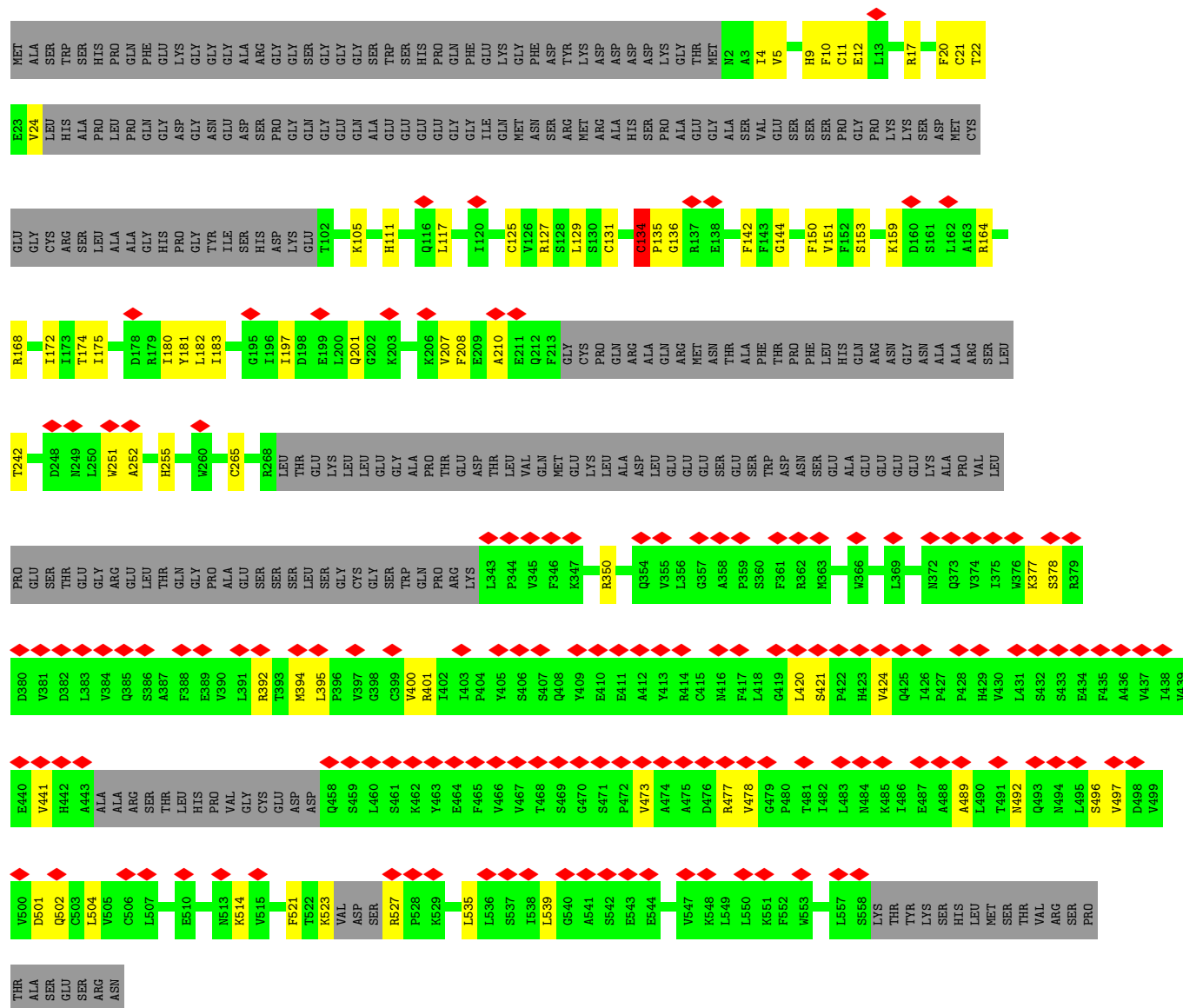
• Molecule 9: Folliculin-interacting protein 2







• Molecule 10: Folliculin



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	177018	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 ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.048	Depositor
Minimum map value	-1.101	Depositor
Average map value	-0.001	Depositor
Map value standard deviation	0.044	Depositor
Recommended contour level	0.48	Depositor
Map size (Å)	461.12, 461.12, 461.12	wwPDB
Map dimensions	440, 440, 440	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.048, 1.048, 1.048	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BEF, CZC, GDP

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	0.32	0/2538	0.60	0/3426
2	B	0.23	0/2333	0.59	0/3138
3	C	0.14	0/727	0.46	1/987 (0.1%)
4	D	0.22	0/914	0.60	0/1236
5	E	0.24	0/918	0.60	0/1245
6	F	0.12	0/705	0.33	0/951
7	G	0.17	0/654	0.49	0/884
8	H	0.26	0/479	0.70	0/656
9	I	0.25	0/3177	0.58	0/4288
10	J	0.26	0/2954	0.55	0/3997
All	All	0.25	0/15399	0.57	1/20808 (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
1	A	0	1
10	J	0	2
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	118	VAL	N-CA-C	-6.11	106.78	112.83

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	72	SER	Peptide
10	J	125	CYS	Peptide
10	J	134	CYS	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	2486	0	2463	75	0
2	B	2291	0	2288	54	0
3	C	717	0	737	11	0
4	D	905	0	921	20	0
5	E	901	0	933	19	0
6	F	696	0	702	10	0
7	G	649	0	649	12	0
8	H	466	0	458	10	0
9	I	3115	0	3160	60	0
10	J	2885	0	2898	51	0
11	A	28	0	0	10	0
12	A	4	0	0	1	0
13	B	28	0	12	0	0
All	All	15171	0	15221	290	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 10.

All (290) 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:181:ASN:OD1	1:A:219:SER:CB	1.68	1.39
1:A:181:ASN:OD1	1:A:219:SER:HB3	1.13	1.27
1:A:181:ASN:CG	1:A:219:SER:HB3	1.79	1.07
1:A:181:ASN:OD1	1:A:219:SER:HB2	1.69	0.89
1:A:179:LYS:HG2	11:A:501:CZC:C9	2.05	0.85
10:J:4:ILE:HG23	10:J:175:ILE:HG23	1.60	0.82
10:J:9:HIS:HE2	10:J:11:CYS:HG	1.30	0.79
1:A:178:HIS:NE2	11:A:501:CZC:O6	2.16	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:313:ILE:HD11	9:I:346:ARG:HH22	1.51	0.76
1:A:179:LYS:HG2	11:A:501:CZC:N1	2.00	0.75
3:C:88:TYR:HA	3:C:91:ARG:HG2	1.72	0.71
1:A:78:GLN:HE21	1:A:114:ILE:HG23	1.56	0.71
10:J:9:HIS:NE2	10:J:11:CYS:SG	2.65	0.70
5:E:53:PHE:HB3	5:E:71:ILE:HD12	1.74	0.69
2:B:197:ILE:O	4:D:3:ARG:NH1	2.27	0.68
9:I:510:GLN:HE21	9:I:513:LEU:HD22	1.60	0.67
1:A:328:LEU:HD11	1:A:336:ALA:HB1	1.77	0.66
1:A:253:ASN:HD21	3:C:65:ILE:HG22	1.61	0.66
8:H:53:VAL:HG13	8:H:54:ILE:HD12	1.77	0.65
2:B:198:ILE:HA	4:D:3:ARG:HH12	1.60	0.65
2:B:202:GLU:HB3	2:B:275:VAL:HB	1.79	0.65
4:D:11:LEU:HB3	4:D:35:SER:HB2	1.79	0.65
10:J:4:ILE:HD11	10:J:21:CYS:HB3	1.79	0.65
4:D:111:LEU:O	4:D:115:LEU:HB2	1.96	0.65
5:E:21:ALA:HB3	5:E:93:ILE:HB	1.78	0.65
1:A:253:ASN:HB2	3:C:67:ASP:HA	1.79	0.64
9:I:48:ARG:HB3	9:I:316:ILE:HB	1.78	0.64
2:B:160:PHE:HB3	2:B:172:ALA:HB1	1.80	0.64
9:I:344:MET:SD	9:I:984:HIS:NE2	2.72	0.63
2:B:266:PHE:HB3	2:B:270:THR:HG23	1.80	0.63
2:B:163:SER:H	2:B:169:LEU:HB2	1.63	0.62
2:B:240:LEU:HD21	8:H:74:LEU:HB3	1.81	0.62
9:I:492:TYR:OH	9:I:958:ASP:OD1	2.17	0.62
6:F:14:ASP:HB3	6:F:90:GLN:HB2	1.82	0.61
9:I:503:ARG:HH22	9:I:959:LEU:H	1.48	0.61
2:B:263:ILE:HG12	2:B:273:MET:HG2	1.82	0.61
1:A:179:LYS:HG2	11:A:501:CZC:C1	2.31	0.61
6:F:56:HIS:ND1	6:F:59:MET:SD	2.73	0.60
9:I:491:LEU:HD21	9:I:960:VAL:HG22	1.83	0.60
1:A:316:ALA:HB3	1:A:328:LEU:HB3	1.82	0.60
7:G:92:GLU:HA	7:G:95:MET:HE2	1.82	0.60
10:J:153:SER:HA	10:J:172:ILE:O	2.01	0.60
8:H:42:ILE:HG12	8:H:44:PRO:HD3	1.84	0.60
1:A:194:ASP:OD2	1:A:198:ARG:NH2	2.34	0.59
1:A:99:ILE:H	1:A:118:PRO:HD3	1.65	0.59
2:B:121:LYS:HG3	2:B:156:GLU:HB3	1.83	0.59
1:A:284:LEU:HG	1:A:326:LEU:HD21	1.85	0.59
7:G:91:LEU:O	7:G:94:THR:OG1	2.20	0.59
1:A:331:VAL:O	1:A:364:HIS:NE2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:288:MET:HE1	1:A:328:LEU:HB2	1.85	0.58
3:C:83:ASP:O	3:C:86:ARG:NH1	2.36	0.58
6:F:55:LEU:H	6:F:62:PRO:HG3	1.68	0.58
10:J:151:VAL:HA	10:J:174:THR:O	2.03	0.58
9:I:428:ILE:HG12	9:I:434:PHE:HB3	1.86	0.58
1:A:193:ARG:NH1	1:A:197:GLN:OE1	2.37	0.58
1:A:263:ASP:OD2	1:A:266:SER:OG	2.22	0.57
2:B:26:ILE:HD13	8:H:74:LEU:HD21	1.86	0.57
4:D:19:VAL:HB	4:D:103:MET:HE1	1.85	0.57
9:I:46:GLU:HB2	9:I:318:SER:HB2	1.87	0.56
10:J:111:HIS:HB2	10:J:117:LEU:HB3	1.86	0.56
7:G:103:VAL:HG22	7:G:168:VAL:HG12	1.87	0.56
1:A:295:VAL:HG23	2:B:234:ILE:HG21	1.88	0.56
9:I:60:ARG:HG2	9:I:61:GLN:H	1.70	0.56
8:H:52:HIS:O	8:H:54:ILE:N	2.38	0.56
9:I:47:ILE:O	9:I:383:ARG:NH2	2.39	0.56
4:D:72:ILE:HB	4:D:83:ILE:HB	1.87	0.56
4:D:74:MET:HB2	4:D:81:VAL:HB	1.88	0.55
10:J:523:LYS:O	10:J:527:ARG:NH1	2.39	0.55
9:I:1046:LEU:HD12	9:I:1047:PRO:HD2	1.88	0.55
1:A:75:SER:OG	1:A:97:ASN:ND2	2.29	0.55
1:A:298:ILE:HD11	2:B:227:ARG:HD3	1.87	0.55
1:A:179:LYS:HE3	11:A:501:CZC:N2	2.22	0.55
4:D:80:ARG:NH2	4:D:99:VAL:O	2.39	0.54
9:I:353:LYS:HE3	9:I:374:ARG:HB2	1.87	0.54
1:A:73:GLY:HA2	11:A:501:CZC:O8	2.07	0.54
1:A:179:LYS:HG2	11:A:501:CZC:C3	2.37	0.54
2:B:70:MET:O	2:B:73:TYR:HB3	2.08	0.54
10:J:17:ARG:NH1	10:J:242:THR:OG1	2.39	0.54
2:B:206:PHE:HB3	2:B:211:PHE:HA	1.90	0.54
9:I:52:TYR:OH	9:I:135:VAL:O	2.25	0.54
1:A:79:LYS:HG3	1:A:93:LEU:HD21	1.88	0.54
1:A:291:VAL:HG12	2:B:252:MET:HE1	1.87	0.54
10:J:350:ARG:NH2	10:J:489:ALA:O	2.40	0.54
2:B:50:VAL:HG12	2:B:58:LEU:HB3	1.90	0.54
1:A:320:LEU:HA	2:B:249:PHE:HA	1.90	0.54
4:D:80:ARG:HE	4:D:97:GLU:HA	1.73	0.53
1:A:95:SER:HA	10:J:164:ARG:HB2	1.90	0.53
9:I:955:TYR:HB3	9:I:970:LEU:HB3	1.90	0.53
9:I:448:TRP:HB3	9:I:526:ARG:HE	1.74	0.53
2:B:92:PHE:HB2	2:B:126:VAL:HG22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:300:GLY:HA3	2:B:256:ASN:HD21	1.74	0.52
1:A:180:VAL:HG12	1:A:183:LEU:HD12	1.91	0.52
9:I:1062:MET:HA	9:I:1065:LYS:HE3	1.90	0.52
9:I:317:PHE:HE2	9:I:386:ILE:HG21	1.75	0.52
1:A:80:VAL:HG11	1:A:220:ILE:HG23	1.92	0.52
1:A:288:MET:HE2	1:A:326:LEU:HB3	1.91	0.52
6:F:69:VAL:HG13	6:F:74:THR:HG22	1.92	0.52
10:J:20:PHE:HZ	10:J:251:TRP:HB3	1.75	0.52
10:J:252:ALA:O	10:J:255:HIS:ND1	2.43	0.52
4:D:2:LEU:HB3	4:D:122:VAL:HG21	1.91	0.51
10:J:394:MET:HG3	10:J:504:LEU:HD11	1.91	0.51
2:B:15:LYS:O	2:B:20:LYS:NZ	2.44	0.51
9:I:1084:LEU:HD22	9:I:1095:LEU:HB2	1.93	0.51
2:B:148:LEU:O	2:B:152:SER:OG	2.28	0.51
10:J:350:ARG:NH2	10:J:492:ASN:O	2.43	0.51
2:B:13:MET:O	2:B:91:VAL:N	2.38	0.51
6:F:11:ARG:NH1	6:F:11:ARG:O	2.44	0.51
7:G:104:LEU:HD13	7:G:124:ALA:HB3	1.92	0.50
6:F:57:ARG:HH21	7:G:120:SER:HB2	1.77	0.50
10:J:197:ILE:O	10:J:201:GLN:HB2	2.11	0.50
1:A:178:HIS:CD2	11:A:501:CZC:O6	2.64	0.50
5:E:68:ASN:ND2	5:E:70:SER:O	2.42	0.50
10:J:12:GLU:OE1	10:J:17:ARG:NH1	2.45	0.50
5:E:18:GLY:HA3	5:E:98:ALA:HB2	1.93	0.50
4:D:53:TRP:HE3	4:D:83:ILE:HG22	1.76	0.50
2:B:251:SER:HA	2:B:263:ILE:O	2.11	0.49
2:B:9:LYS:HG3	2:B:85:VAL:HG23	1.94	0.49
3:C:91:ARG:HH21	5:E:121:VAL:HG23	1.75	0.49
1:A:244:GLU:O	1:A:248:ASN:ND2	2.46	0.49
9:I:979:VAL:HA	9:I:982:VAL:HG12	1.94	0.49
9:I:341:GLU:HG2	9:I:986:VAL:HG22	1.94	0.49
2:B:28:PHE:HE2	2:B:50:VAL:HG13	1.78	0.49
3:C:49:ASP:N	3:C:49:ASP:OD1	2.46	0.49
9:I:141:MET:HG2	10:J:134:CYS:HB3	1.95	0.49
1:A:291:VAL:HG13	2:B:234:ILE:HG22	1.95	0.49
3:C:57:ILE:HG13	3:C:60:LYS:HE3	1.94	0.49
4:D:24:LEU:HB3	4:D:33:ALA:HB3	1.95	0.48
9:I:399:VAL:HG12	9:I:522:THR:HG23	1.95	0.48
9:I:504:THR:HG22	9:I:997:ILE:HG22	1.93	0.48
1:A:312:LYS:HE3	1:A:360:ARG:HH22	1.78	0.48
10:J:24:VAL:HB	10:J:105:LYS:HG3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ASN:HB2	8:H:72:SER:HB2	1.95	0.48
1:A:181:ASN:ND2	1:A:219:SER:HB3	2.27	0.48
1:A:342:ARG:O	1:A:346:PHE:N	2.45	0.48
9:I:333:PHE:CD1	9:I:339:LEU:HD13	2.48	0.48
9:I:980:HIS:HA	9:I:983:HIS:CE1	2.49	0.48
2:B:171:LYS:NZ	2:B:225:VAL:O	2.38	0.48
7:G:93:ASP:O	7:G:96:LYS:HB2	2.13	0.47
7:G:143:ASP:N	7:G:143:ASP:OD1	2.46	0.47
9:I:167:MET:HG3	9:I:316:ILE:HD13	1.96	0.47
5:E:47:PRO:O	5:E:51:SER:HB3	2.14	0.47
5:E:61:SER:HA	5:E:67:LYS:HG2	1.96	0.47
9:I:353:LYS:O	9:I:374:ARG:NH2	2.47	0.47
3:C:111:LEU:HD12	6:F:64:LYS:HB3	1.96	0.47
1:A:248:ASN:ND2	1:A:274:SER:OG	2.47	0.47
2:B:210:THR:HB	2:B:212:LEU:HD13	1.97	0.47
3:C:132:VAL:HG21	7:G:157:MET:HE1	1.95	0.47
7:G:90:HIS:O	7:G:93:ASP:HB2	2.14	0.47
9:I:1002:ASP:OD1	9:I:1003:LYS:N	2.47	0.47
5:E:107:GLU:HA	5:E:110:LEU:HB2	1.95	0.47
9:I:53:GLN:HB2	9:I:60:ARG:HE	1.79	0.47
9:I:141:MET:HE2	10:J:135:PRO:HA	1.95	0.47
10:J:477:ARG:HG3	10:J:478:VAL:HG13	1.96	0.47
1:A:220:ILE:HA	1:A:225:ILE:HD13	1.97	0.47
2:B:100:GLU:HA	2:B:103:MET:HG2	1.95	0.47
9:I:988:ASP:OD1	9:I:989:GLU:N	2.47	0.47
10:J:180:ILE:HA	10:J:183:ILE:HG12	1.96	0.47
2:B:101:LYS:NZ	2:B:105:TYR:OH	2.46	0.47
10:J:181:TYR:OH	10:J:265:CYS:O	2.22	0.47
6:F:77:VAL:HG22	6:F:86:VAL:HG13	1.96	0.46
9:I:49:LEU:HD11	9:I:346:ARG:NH2	2.31	0.46
2:B:127:HIS:CE1	2:B:164:ILE:HG23	2.50	0.46
1:A:174:GLU:HG2	1:A:232:VAL:HG22	1.97	0.46
1:A:233:VAL:O	1:A:237:ILE:HG13	2.16	0.46
9:I:393:PRO:HG2	9:I:950:GLY:HA3	1.96	0.46
5:E:38:ASP:OD1	5:E:38:ASP:N	2.49	0.46
1:A:298:ILE:HD13	2:B:231:ILE:HG12	1.98	0.46
2:B:27:ILE:HD13	2:B:236:LYS:HZ1	1.81	0.46
9:I:428:ILE:HG22	9:I:432:GLN:HA	1.98	0.46
1:A:273:ASP:OD2	1:A:275:SER:OG	2.26	0.45
9:I:171:VAL:HG13	9:I:312:ALA:HB2	1.98	0.45
9:I:49:LEU:HB2	9:I:379:LEU:HD13	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:12:GLU:HB2	10:J:17:ARG:HH11	1.82	0.45
1:A:154:LEU:HD23	1:A:157:LEU:HD23	1.98	0.45
7:G:159:GLN:NE2	7:G:166:VAL:O	2.50	0.45
1:A:349:LYS:NZ	1:A:353:ASP:HB2	2.31	0.45
9:I:50:ILE:HG13	9:I:138:LEU:HD23	1.98	0.45
9:I:440:ALA:HA	9:I:443:THR:HG22	1.97	0.45
3:C:84:ARG:NH2	5:E:26:ASP:OD2	2.49	0.45
6:F:77:VAL:HA	6:F:85:PHE:O	2.16	0.45
2:B:27:ILE:HD12	2:B:212:LEU:HD11	1.99	0.45
1:A:203:LEU:HD11	1:A:211:LEU:HD12	1.98	0.45
4:D:4:PRO:HA	4:D:7:LEU:HD13	1.99	0.45
5:E:105:SER:HA	5:E:108:LYS:HB2	1.99	0.45
10:J:21:CYS:HB2	10:J:111:HIS:H	1.82	0.45
1:A:192:GLN:HB2	1:A:217:LEU:HD21	1.98	0.45
2:B:29:ALA:HB2	2:B:236:LYS:HG2	1.99	0.44
10:J:197:ILE:O	10:J:201:GLN:CB	2.66	0.44
1:A:296:SER:OG	2:B:256:ASN:ND2	2.43	0.44
3:C:92:LEU:HD11	5:E:33:ILE:HD12	1.99	0.44
1:A:139:ALA:HB2	1:A:236:LEU:HD21	1.98	0.44
1:A:142:TYR:CE2	1:A:157:LEU:HB2	2.52	0.44
1:A:329:LYS:HB3	1:A:329:LYS:HE3	1.79	0.44
4:D:67:ASP:OD2	5:E:76:ASN:ND2	2.48	0.44
10:J:496:SER:OG	10:J:497:VAL:N	2.50	0.44
1:A:195:ILE:HG22	1:A:215:PHE:HE2	1.82	0.44
5:E:17:GLU:OE1	7:G:133:GLN:NE2	2.51	0.44
2:B:96:SER:HB2	2:B:101:LYS:HB3	2.00	0.44
1:A:78:GLN:NE2	1:A:114:ILE:O	2.50	0.44
1:A:296:SER:OG	1:A:309:ALA:O	2.27	0.44
2:B:12:LEU:HD13	2:B:89:ILE:HB	2.00	0.44
4:D:23:LEU:O	4:D:91:LEU:HA	2.18	0.44
10:J:10:PHE:HD1	10:J:129:LEU:HG	1.82	0.44
8:H:61:ALA:O	8:H:65:ASN:N	2.48	0.43
9:I:47:ILE:HD12	9:I:383:ARG:HG3	2.00	0.43
9:I:452:VAL:O	9:I:453:MET:HE2	2.18	0.43
1:A:69:LEU:HD21	1:A:156:ARG:HG3	2.00	0.43
10:J:514:LYS:HG2	10:J:539:LEU:HD13	2.00	0.43
1:A:138:GLY:HA3	1:A:236:LEU:HD11	1.99	0.43
10:J:392:ARG:HG3	10:J:400:VAL:HG21	2.00	0.43
2:B:249:PHE:HE2	2:B:252:MET:HB2	1.84	0.43
5:E:107:GLU:HB3	5:E:114:PHE:HE2	1.84	0.43
2:B:259:PHE:HA	2:B:277:SER:HA	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:39:PRO:HB3	8:H:91:ALA:HA	2.00	0.43
10:J:378:SER:HA	10:J:441:VAL:HB	2.01	0.43
1:A:230:SER:O	1:A:234:GLN:CB	2.67	0.43
9:I:1046:LEU:HD13	10:J:521:PHE:HE1	1.84	0.43
1:A:97:ASN:OD1	12:A:502:BEF:F2	2.27	0.43
2:B:70:MET:O	2:B:73:TYR:CB	2.66	0.43
10:J:142:PHE:HE1	10:J:182:LEU:HD23	1.83	0.43
10:J:400:VAL:O	10:J:401:ARG:NE	2.52	0.43
10:J:420:LEU:HD22	10:J:424:VAL:HG11	2.01	0.43
2:B:127:HIS:CG	2:B:128:LYS:H	2.36	0.43
10:J:127:ARG:HA	10:J:131:CYS:HB3	2.01	0.43
1:A:230:SER:O	1:A:234:GLN:HB2	2.18	0.43
9:I:449:VAL:HG23	9:I:450:PRO:HD3	2.01	0.43
1:A:100:TYR:HB3	1:A:116:ASP:HB2	2.01	0.43
2:B:126:VAL:HG11	2:B:144:ARG:HD3	2.00	0.43
4:D:76:CYS:SG	4:D:77:MET:N	2.92	0.43
1:A:203:LEU:HD21	1:A:211:LEU:HB2	2.01	0.42
9:I:422:THR:HA	9:I:425:ILE:HG12	2.01	0.42
9:I:488:LEU:HD13	9:I:943:PHE:CZ	2.54	0.42
2:B:132:VAL:HG13	2:B:136:GLN:NE2	2.34	0.42
1:A:292:VAL:HG21	1:A:316:ALA:HB2	2.01	0.42
2:B:187:LEU:HD22	2:B:300:LEU:HD23	2.01	0.42
5:E:88:LEU:HD21	5:E:121:VAL:HG13	2.01	0.42
9:I:503:ARG:NH1	9:I:958:ASP:HA	2.34	0.42
1:A:179:LYS:HD2	11:A:501:CZC:C2	2.49	0.42
5:E:28:ASP:N	5:E:28:ASP:OD1	2.52	0.42
9:I:340:PHE:CZ	10:J:183:ILE:HD12	2.55	0.42
9:I:503:ARG:NH1	9:I:959:LEU:O	2.49	0.42
9:I:954:THR:OG1	9:I:955:TYR:N	2.50	0.42
5:E:34:LYS:HE2	5:E:34:LYS:HB2	1.89	0.42
10:J:377:LYS:NZ	10:J:424:VAL:O	2.47	0.42
1:A:177:ILE:HD11	1:A:215:PHE:HD2	1.83	0.42
1:A:337:LEU:HD22	1:A:359:PHE:CE2	2.55	0.42
10:J:395:LEU:HD23	10:J:400:VAL:HA	2.02	0.42
9:I:385:THR:HG22	9:I:957:PRO:HG3	2.01	0.42
10:J:134:CYS:O	10:J:136:GLY:N	2.52	0.42
2:B:18:SER:OG	2:B:20:LYS:NZ	2.46	0.42
2:B:164:ILE:O	8:H:71:TYR:OH	2.31	0.42
9:I:130:ARG:NH1	9:I:131:PRO:O	2.53	0.42
9:I:336:HIS:HB3	9:I:338:PRO:HD2	2.02	0.42
2:B:173:TRP:HD1	2:B:176:ILE:HD12	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:53:TRP:HB3	4:D:90:LEU:HD11	2.02	0.41
4:D:81:VAL:HG22	4:D:94:TYR:HB3	2.02	0.41
9:I:1038:ILE:HD11	9:I:1051:CYS:SG	2.60	0.41
1:A:101:LYS:HE3	1:A:115:TRP:CZ2	2.55	0.41
9:I:169:SER:HB3	9:I:314:SER:HB2	2.02	0.41
10:J:521:PHE:HE2	10:J:535:LEU:HD13	1.85	0.41
4:D:92:CYS:SG	4:D:93:MET:N	2.93	0.41
2:B:27:ILE:HG13	2:B:173:TRP:CZ3	2.55	0.41
2:B:162:THR:HA	2:B:169:LEU:HD13	2.03	0.41
9:I:1038:ILE:HD12	9:I:1041:LEU:HB3	2.01	0.41
10:J:159:LYS:HB3	10:J:208:PHE:CG	2.54	0.41
4:D:23:LEU:HD13	4:D:46:ALA:HB1	2.03	0.41
6:F:11:ARG:HA	6:F:11:ARG:HD2	1.86	0.41
10:J:142:PHE:CE1	10:J:182:LEU:HD23	2.55	0.41
10:J:5:VAL:O	10:J:21:CYS:HA	2.20	0.41
2:B:26:ILE:HD13	2:B:26:ILE:HA	1.96	0.41
1:A:75:SER:HG	1:A:97:ASN:HD21	1.61	0.41
1:A:77:ILE:O	1:A:81:VAL:HG22	2.21	0.41
2:B:26:ILE:O	8:H:70:TYR:OH	2.38	0.41
9:I:47:ILE:HG22	9:I:379:LEU:HD11	2.02	0.41
9:I:157:ILE:HB	10:J:142:PHE:HB3	2.03	0.41
9:I:417:PHE:HE1	9:I:520:VAL:HA	1.85	0.41
10:J:5:VAL:HG12	10:J:22:THR:HB	2.03	0.41
1:A:165:TYR:HE1	1:A:169:PRO:HB3	1.86	0.41
2:B:226:HIS:O	2:B:230:LYS:CB	2.69	0.41
9:I:948:LEU:HD13	9:I:960:VAL:HG11	2.03	0.41
10:J:501:ASP:OD1	10:J:502:GLN:N	2.54	0.41
7:G:127:ILE:HD13	7:G:127:ILE:HA	1.95	0.40
9:I:1034:LEU:HD13	9:I:1058:ARG:HG3	2.03	0.40
10:J:377:LYS:NZ	10:J:421:SER:O	2.42	0.40
1:A:314:SER:HA	2:B:255:ARG:O	2.22	0.40
5:E:103:ILE:HA	5:E:106:LEU:HG	2.03	0.40
10:J:144:GLY:HA3	10:J:150:PHE:HA	2.02	0.40
1:A:97:ASN:OD1	11:A:501:CZC:O10	2.39	0.40
10:J:9:HIS:CE1	10:J:168:ARG:HE	2.38	0.40
10:J:207:VAL:HA	10:J:210:ALA:HB3	2.03	0.40

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	302/400 (76%)	278 (92%)	23 (8%)	1 (0%)	36	66
2	B	271/336 (81%)	254 (94%)	17 (6%)	0	100	100
3	C	86/166 (52%)	83 (96%)	3 (4%)	0	100	100
4	D	116/127 (91%)	110 (95%)	6 (5%)	0	100	100
5	E	114/124 (92%)	107 (94%)	7 (6%)	0	100	100
6	F	89/99 (90%)	87 (98%)	2 (2%)	0	100	100
7	G	85/173 (49%)	82 (96%)	3 (4%)	0	100	100
8	H	57/356 (16%)	45 (79%)	10 (18%)	2 (4%)	3	22
9	I	367/1351 (27%)	336 (92%)	30 (8%)	1 (0%)	36	66
10	J	349/622 (56%)	325 (93%)	22 (6%)	2 (1%)	21	55
All	All	1836/3754 (49%)	1707 (93%)	123 (7%)	6 (0%)	37	66

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ILE
8	H	53	VAL
8	H	59	ASP
10	J	134	CYS
10	J	473	VAL
9	I	163	PRO

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	281/341 (82%)	281 (100%)	0	100	100
2	B	258/308 (84%)	258 (100%)	0	100	100
3	C	81/145 (56%)	81 (100%)	0	100	100
4	D	94/98 (96%)	94 (100%)	0	100	100
5	E	101/108 (94%)	101 (100%)	0	100	100
6	F	76/83 (92%)	76 (100%)	0	100	100
7	G	74/140 (53%)	74 (100%)	0	100	100
8	H	53/316 (17%)	53 (100%)	0	100	100
9	I	347/1165 (30%)	347 (100%)	0	100	100
10	J	323/534 (60%)	323 (100%)	0	100	100
All	All	1688/3238 (52%)	1688 (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 (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	78	GLN
1	A	355	ASN
2	B	59	ASN
2	B	237	GLN
2	B	258	ASN
2	B	289	ASN
5	E	79	GLN
8	H	46	ASN
9	I	61	GLN
9	I	388	ASN
9	I	427	GLN
9	I	980	HIS
10	J	114	HIS
10	J	201	GLN
10	J	494	ASN

5.3.3 RNA ⓘ

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](#)

3 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$
13	GDP	B	500	-	29,30,30	1.20	2 (6%)	45,47,47	1.84	6 (13%)
11	CZC	A	501	12	29,30,30	1.67	7 (24%)	40,47,47	1.61	7 (17%)
12	BEF	A	502	11	0,3,3	-	-	-		

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
13	GDP	B	500	-	-	2/16/32/32	0/3/3/3
11	CZC	A	501	12	-	2/16/32/32	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	501	CZC	C2-N4	-3.90	1.33	1.37
13	B	500	GDP	C5-C4	3.15	1.47	1.38
11	A	501	CZC	O1-C1	3.11	1.30	1.23
13	B	500	GDP	C6-N1	-2.74	1.33	1.38
11	A	501	CZC	C3-N3	-2.74	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	501	CZC	C3-C9	-2.63	1.34	1.44
11	A	501	CZC	C3-C2	-2.57	1.34	1.38
11	A	501	CZC	P1-O7	2.28	1.62	1.59
11	A	501	CZC	P2-O10	-2.06	1.47	1.54

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	500	GDP	C5-C4-N3	-6.38	118.24	128.39
11	A	501	CZC	C9-N1-C1	-5.68	118.55	126.37
13	B	500	GDP	C2-N3-C4	5.20	121.25	112.30
13	B	500	GDP	N9-C4-N3	4.59	135.13	125.95
11	A	501	CZC	C3-C2-N4	3.84	108.02	106.25
13	B	500	GDP	C6-C5-N7	3.57	136.79	130.29
13	B	500	GDP	C4-C5-N7	-2.84	106.16	110.67
11	A	501	CZC	N4-C10-N3	-2.82	108.17	113.40
11	A	501	CZC	C3-C9-N1	2.37	119.29	113.25
11	A	501	CZC	N2-C1-N1	2.23	119.25	115.74
11	A	501	CZC	O11-P2-O10	2.21	116.09	107.80
11	A	501	CZC	C10-N3-C3	2.19	108.17	104.26
13	B	500	GDP	C5-C6-N1	2.00	118.35	113.25

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	A	501	CZC	O4-C7-C8-O5
13	B	500	GDP	C5'-O5'-PA-O3A
11	A	501	CZC	C6-C7-C8-O5
13	B	500	GDP	C5'-O5'-PA-O1A

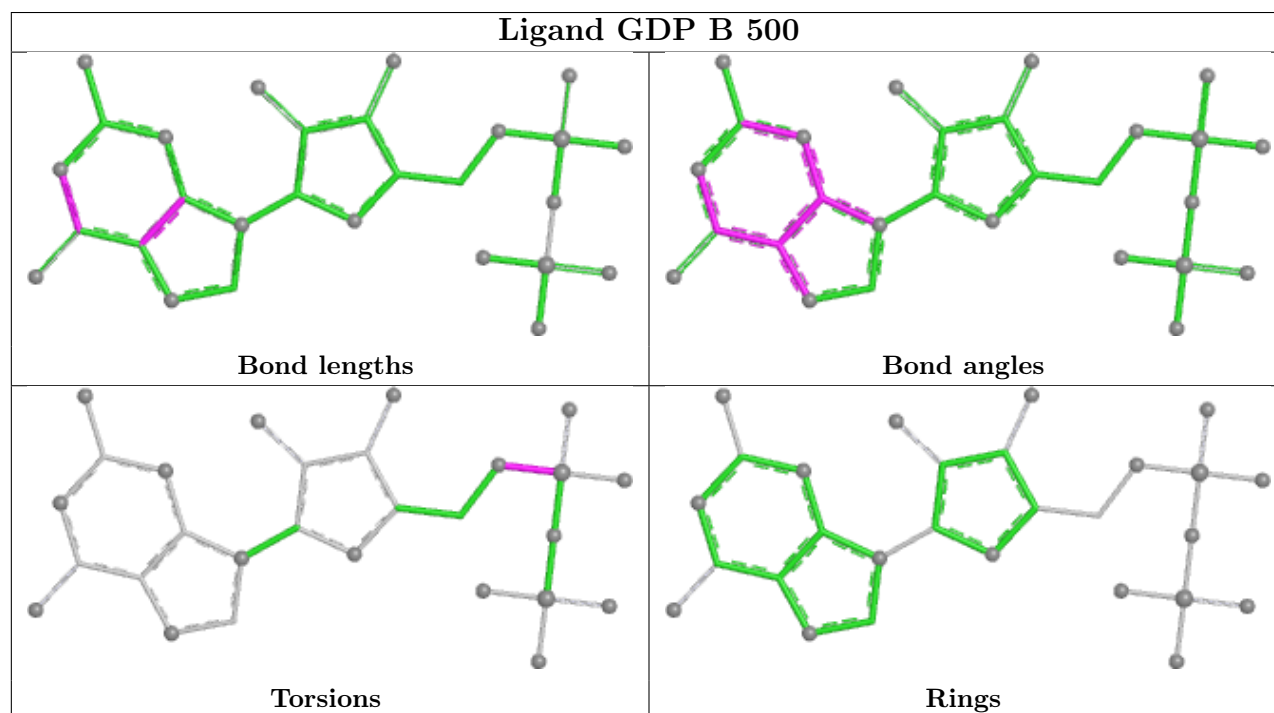
There are no ring outliers.

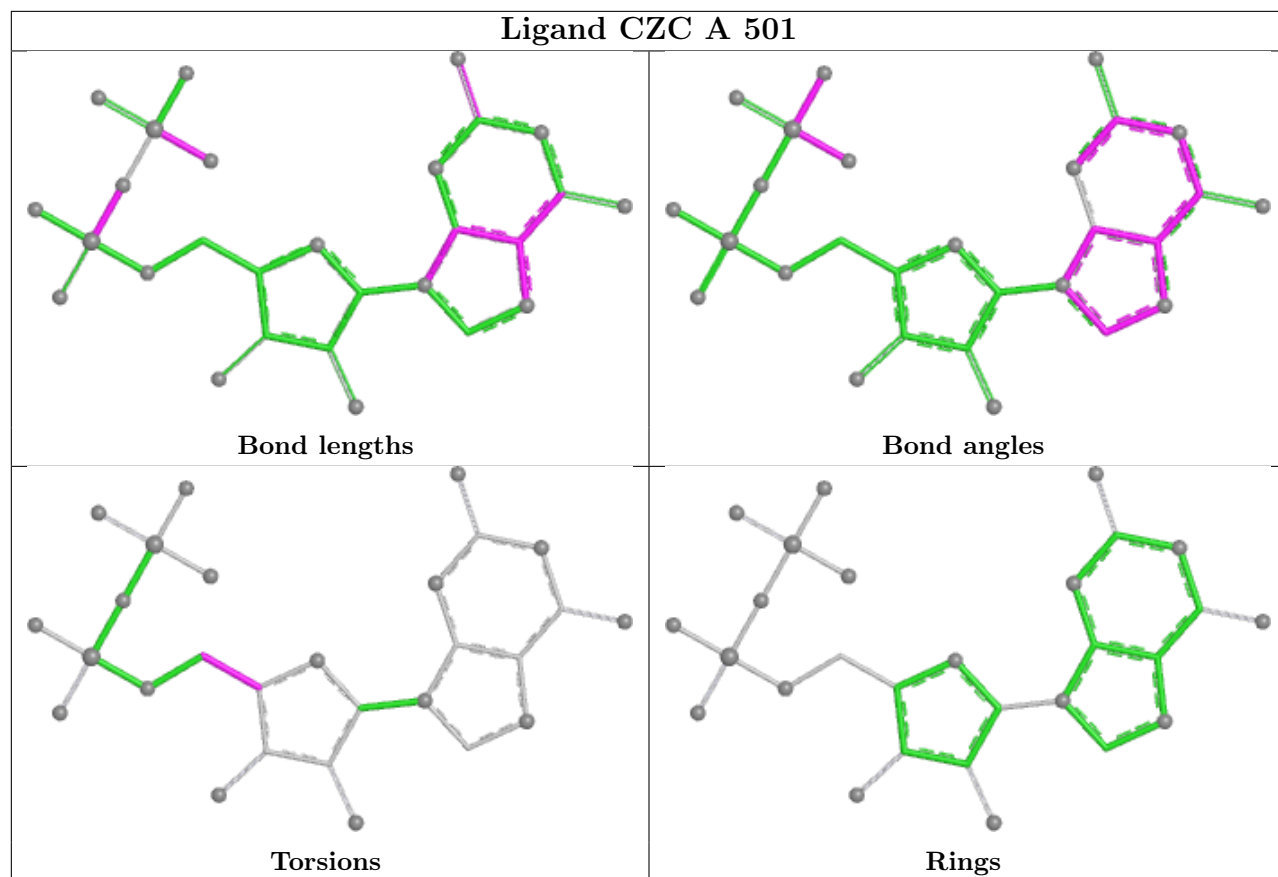
2 monomers are involved in 11 short contacts:

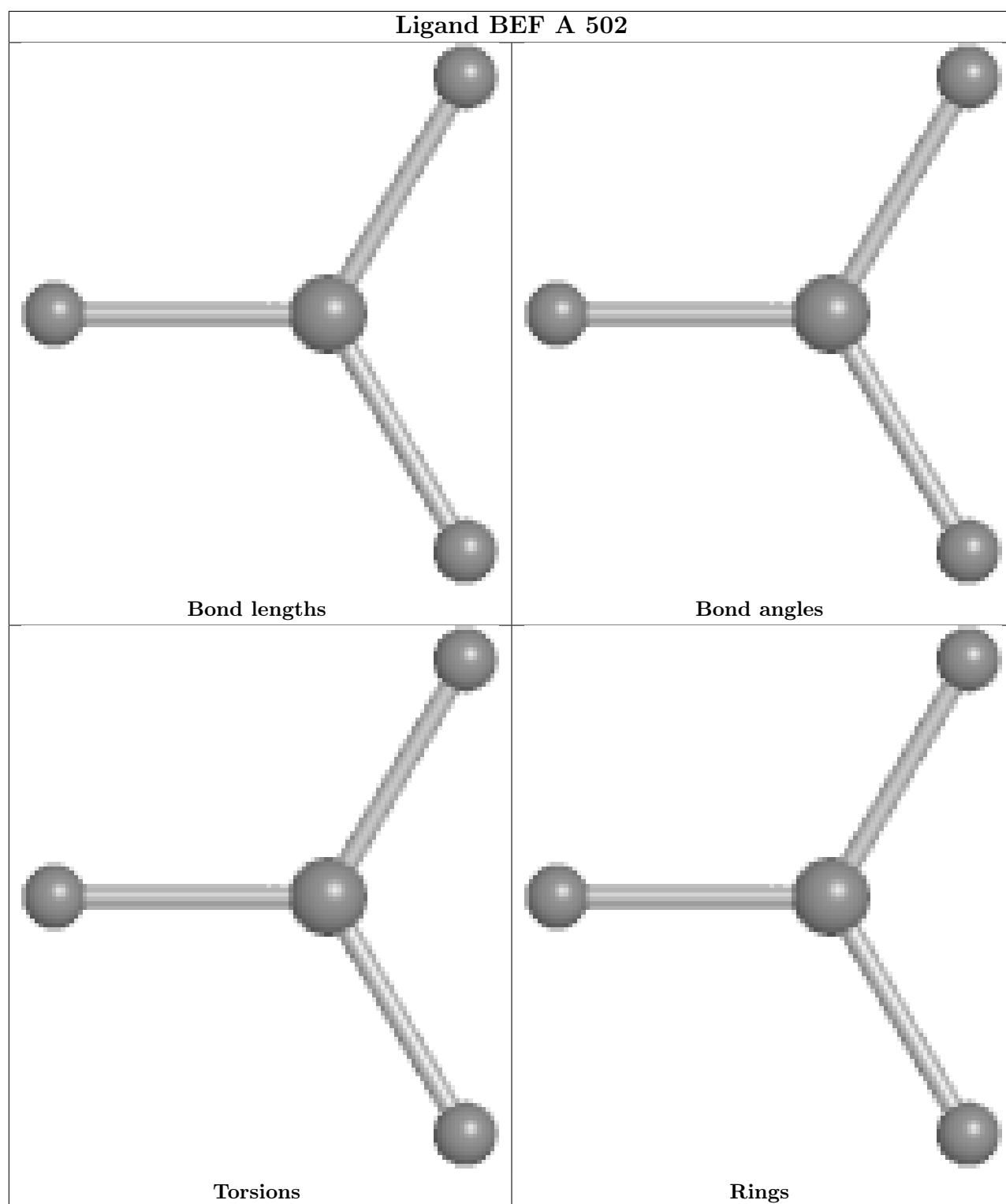
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	A	501	CZC	10	0
12	A	502	BEF	1	0

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 than 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.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

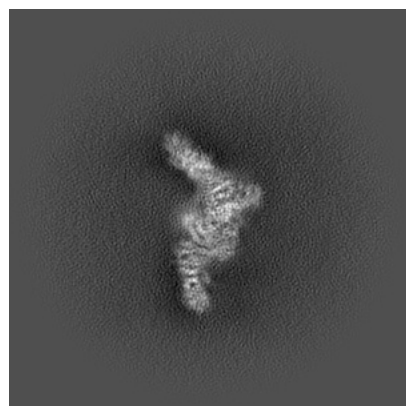
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-27435. These allow visual inspection of the internal detail of the map and identification of artifacts.

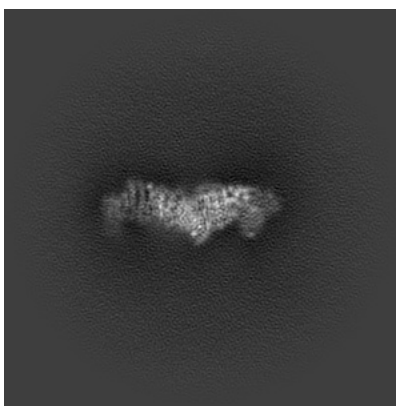
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

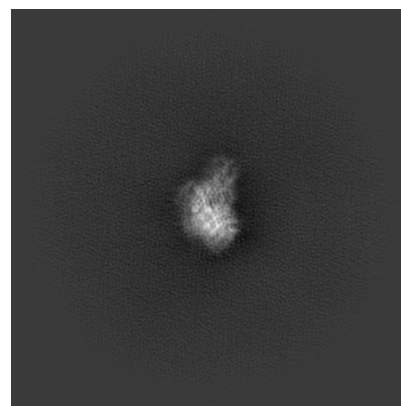
6.1.1 Primary map



X

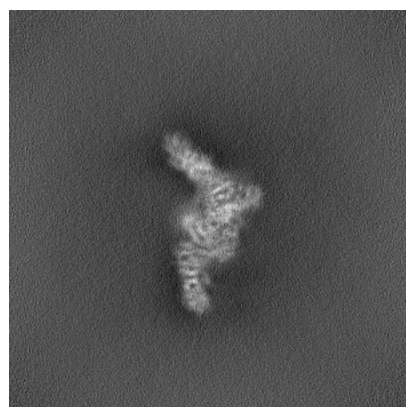


Y

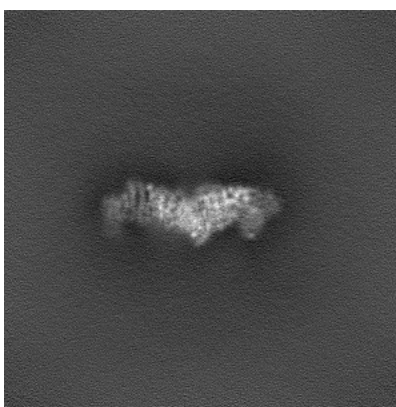


Z

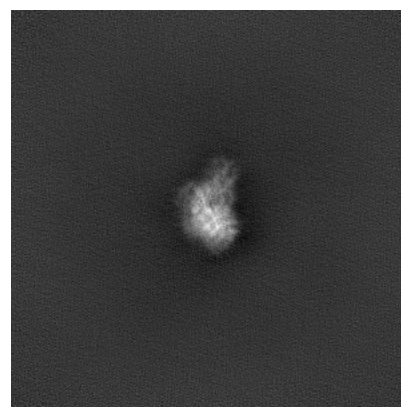
6.1.2 Raw map



X



Y

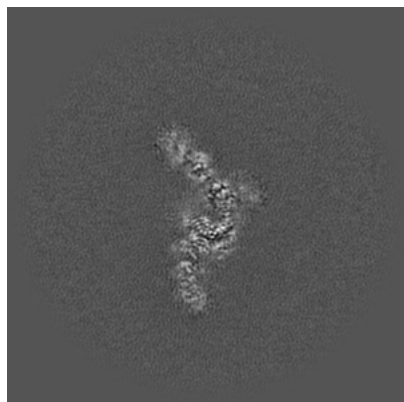


Z

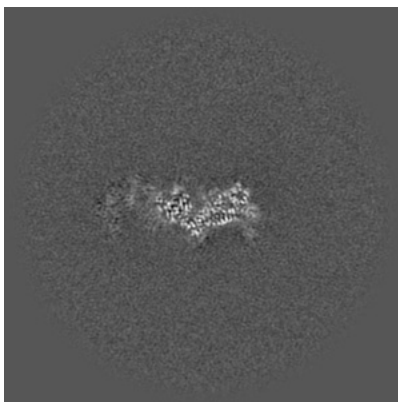
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

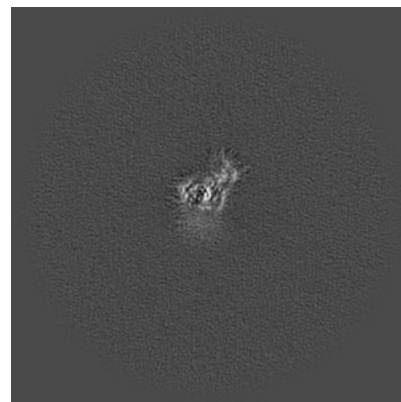
6.2.1 Primary map



X Index: 220



Y Index: 220

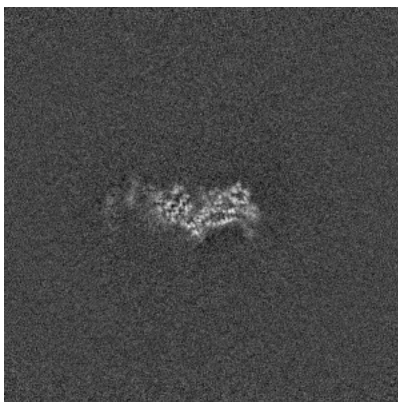


Z Index: 220

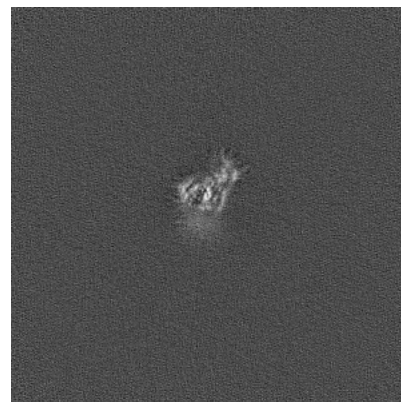
6.2.2 Raw map



X Index: 220



Y Index: 220

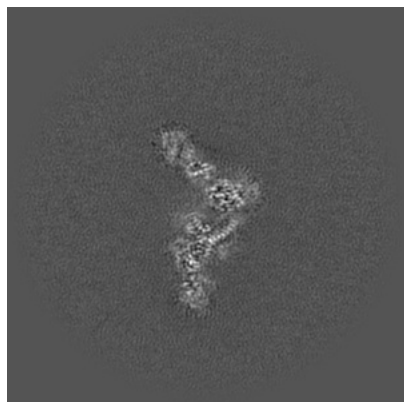


Z Index: 220

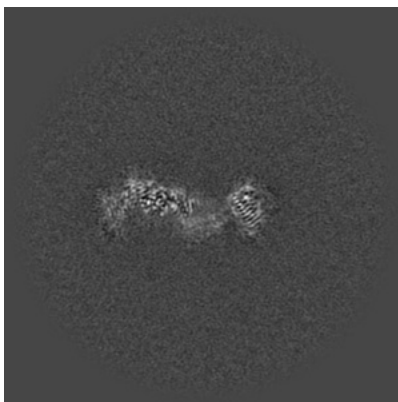
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

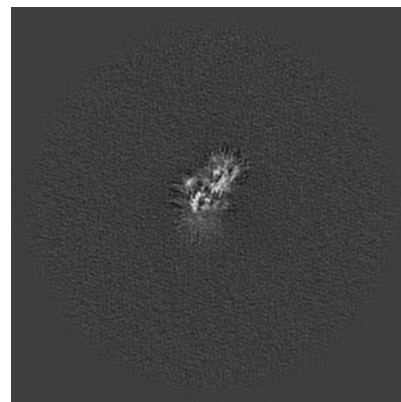
6.3.1 Primary map



X Index: 226

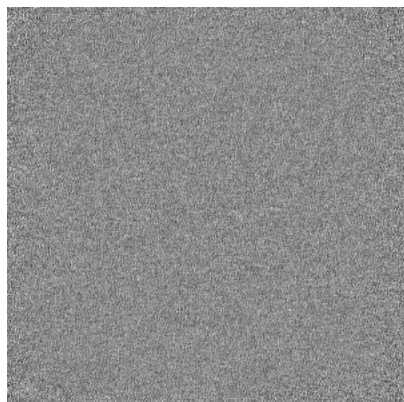


Y Index: 206

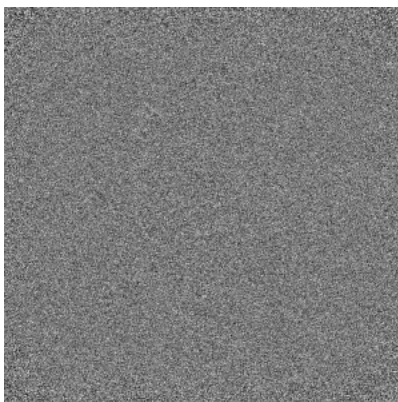


Z Index: 225

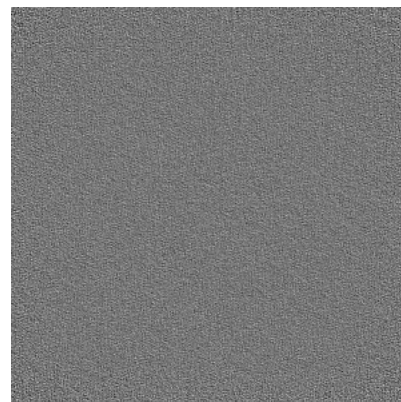
6.3.2 Raw map



X Index: 0



Y Index: 0

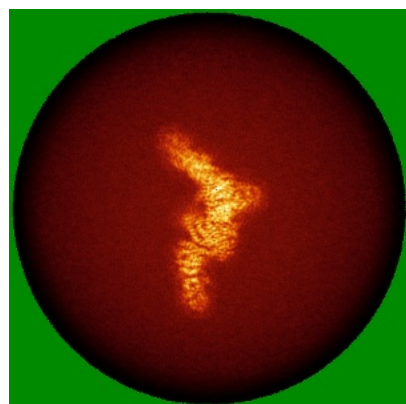


Z Index: 0

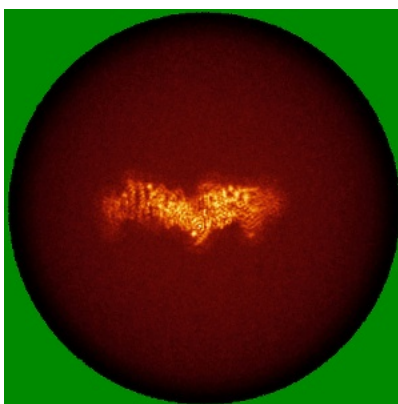
The images above show the largest variance slices of the map in three orthogonal directions.

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

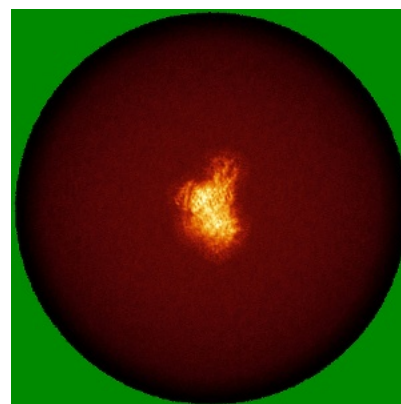
6.4.1 Primary map



X



Y

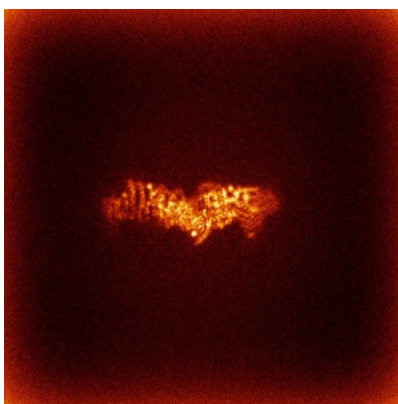


Z

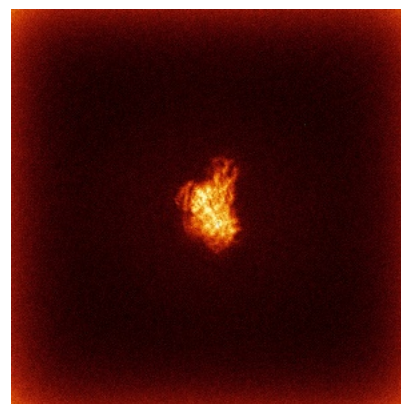
6.4.2 Raw map



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.

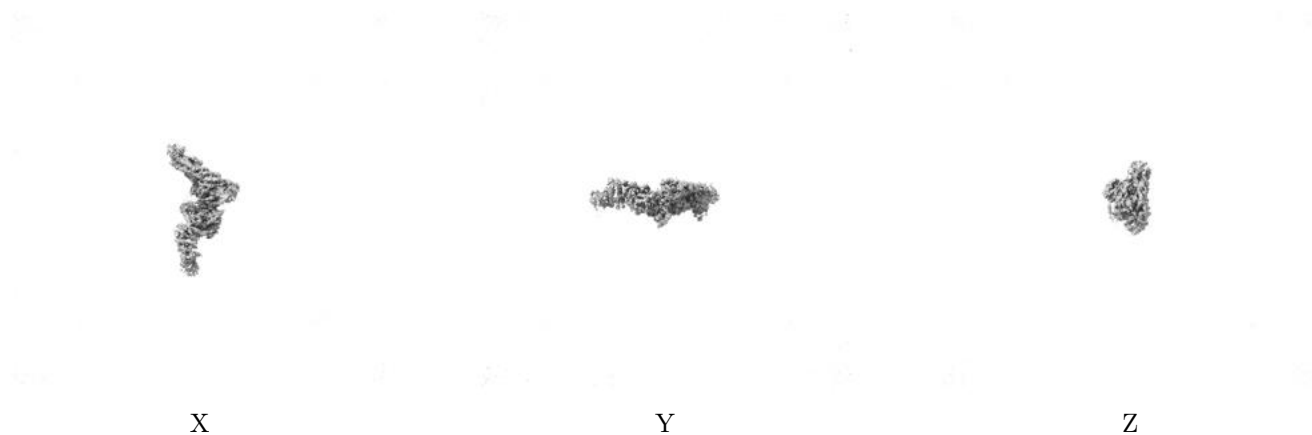
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.48. 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



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.

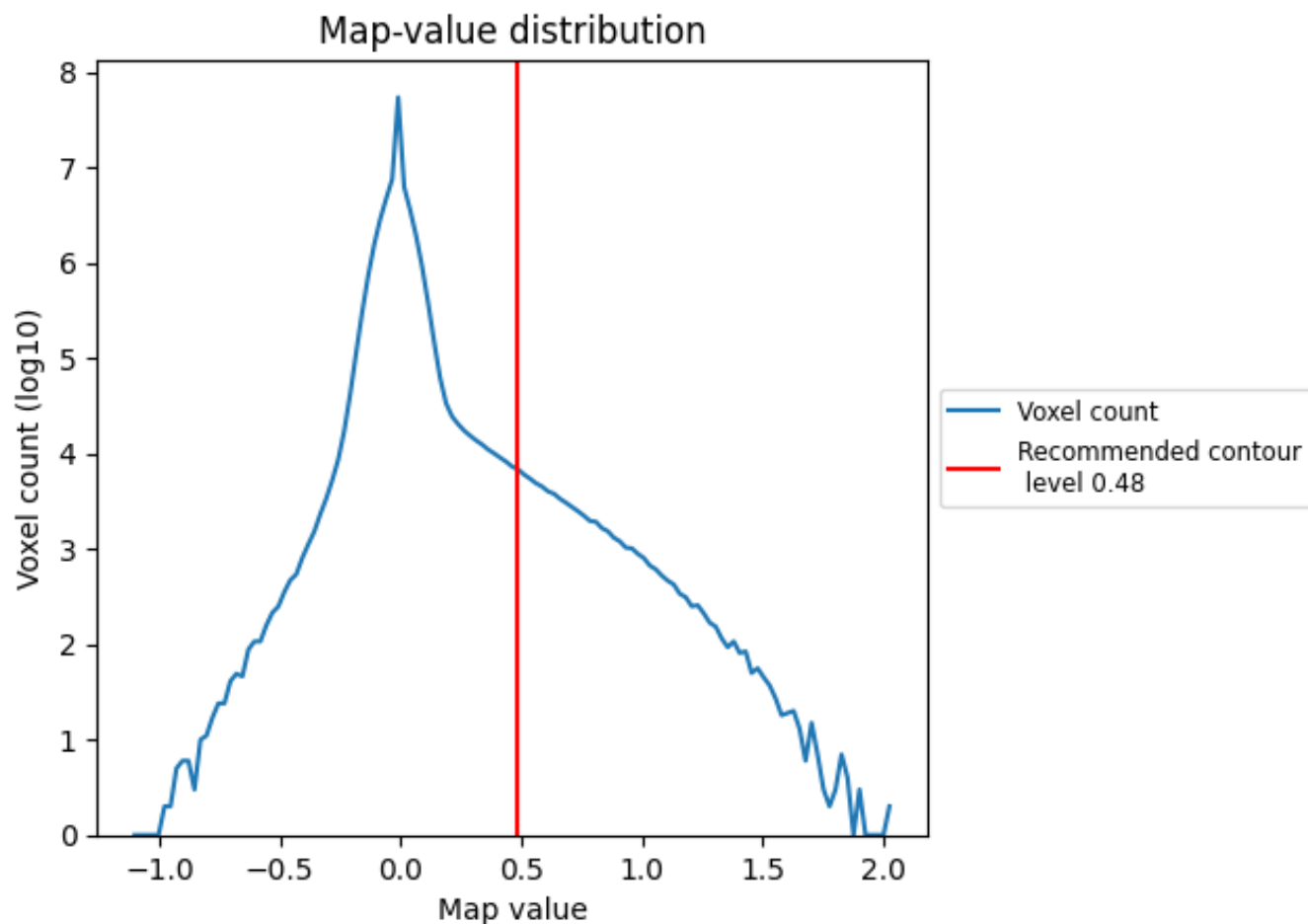
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

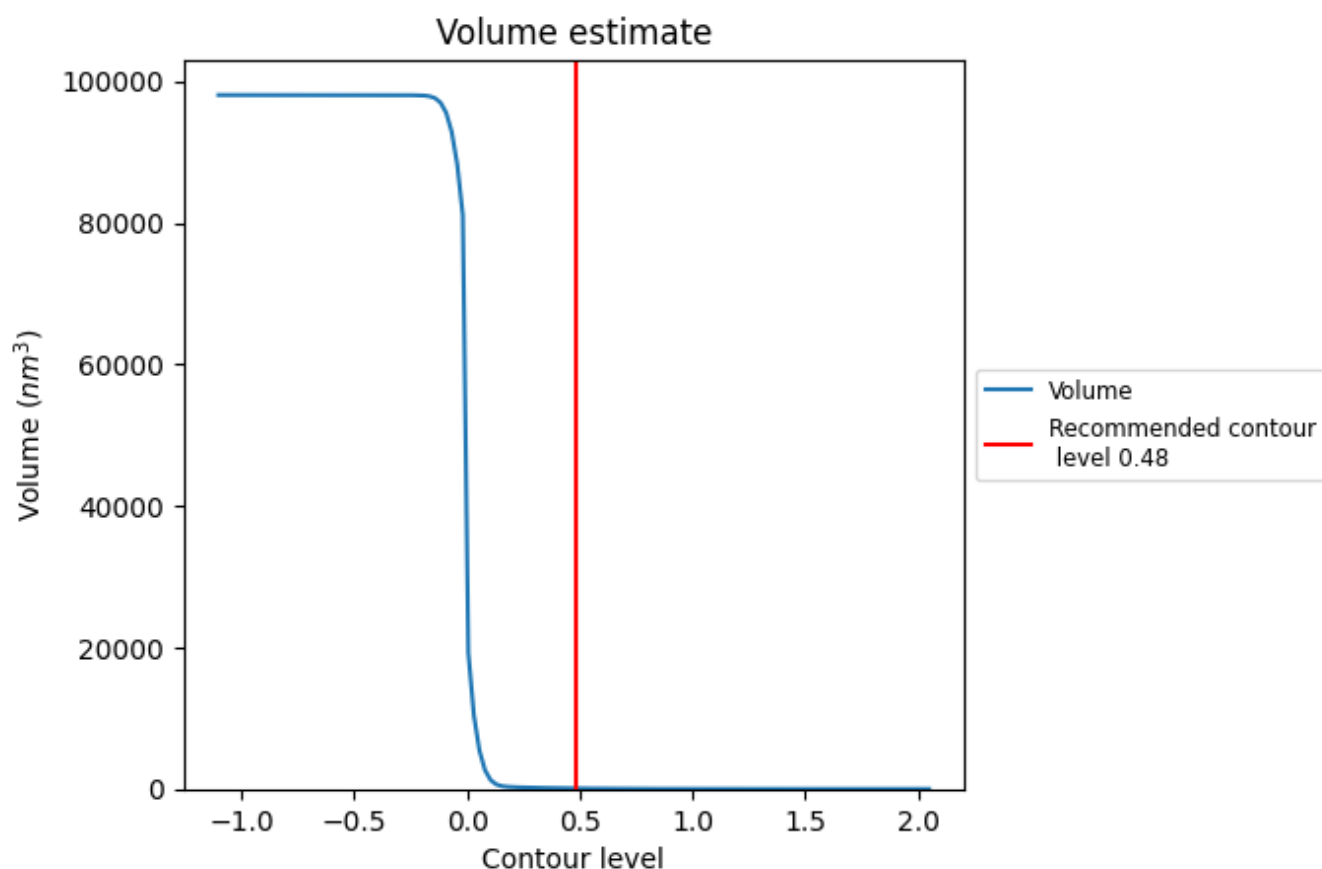
This section contains the results of statistical analysis of the map.

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.

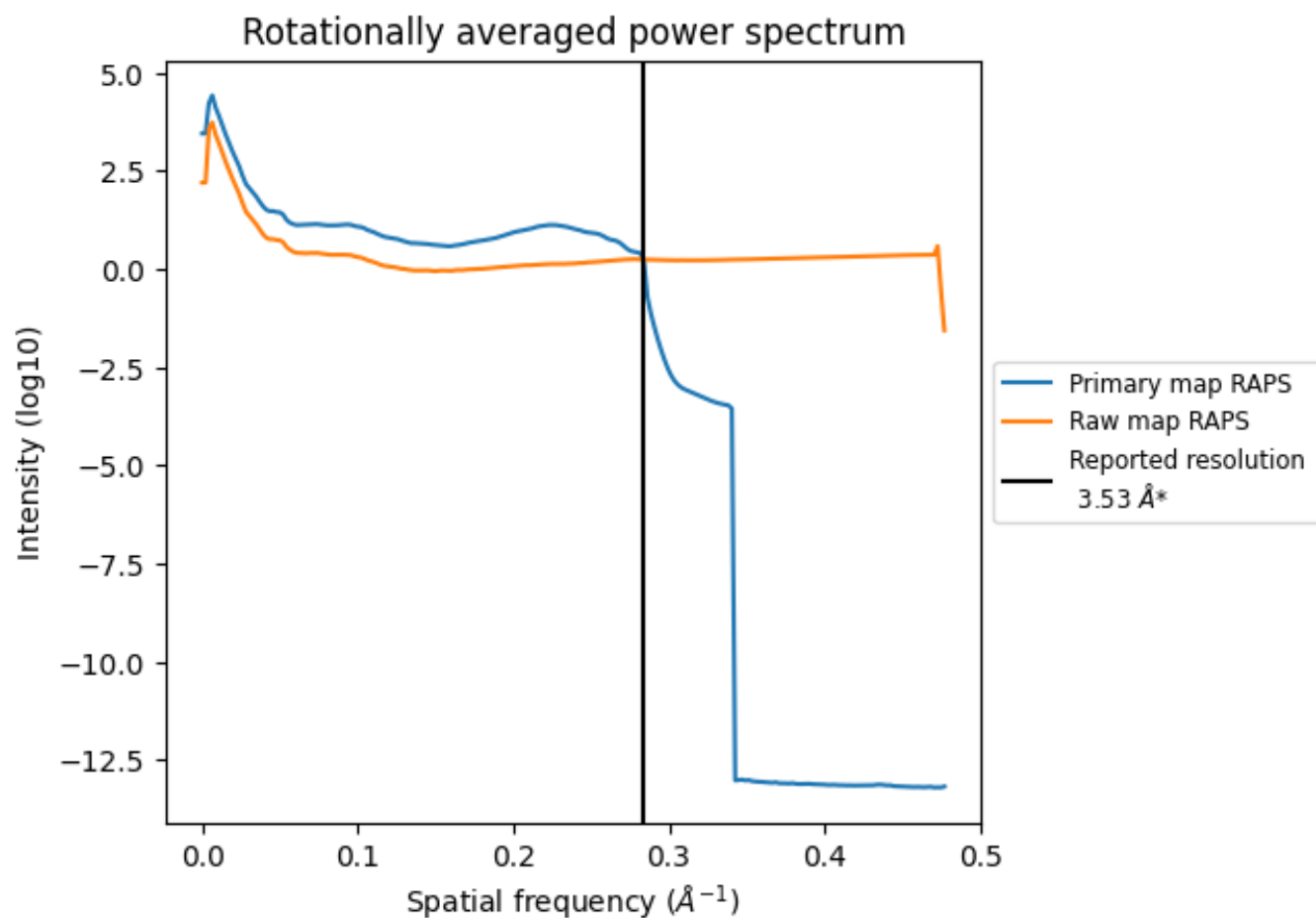
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 80 nm^3 ; this corresponds to an approximate mass of 72 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 ⓘ

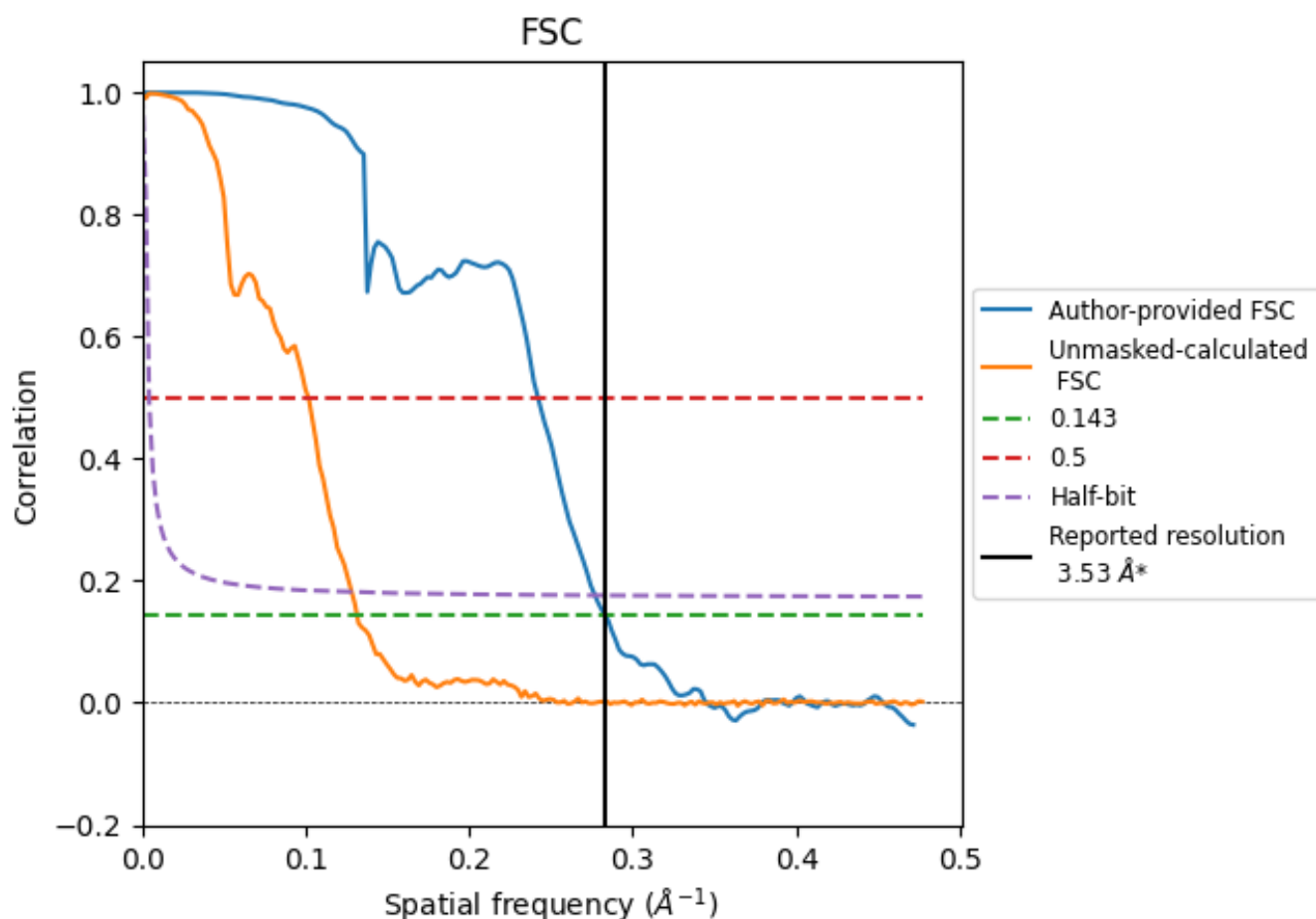


*Reported resolution corresponds to spatial frequency of 0.283 Å⁻¹

8 Fourier-Shell correlation [i](#)

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 [i](#)



*Reported resolution corresponds to spatial frequency of 0.283 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

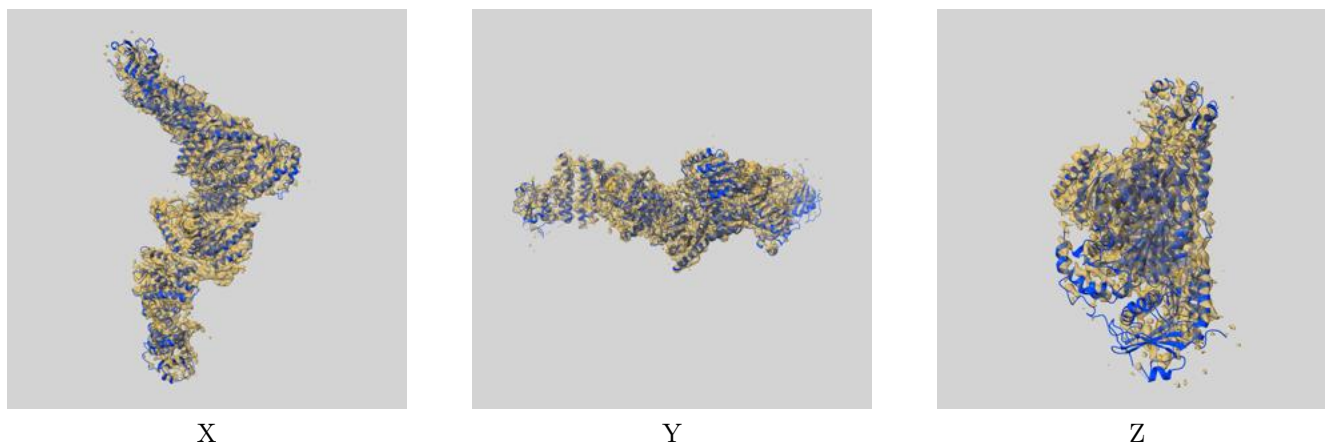
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.53	-	-
Author-provided FSC curve	3.53	4.13	3.61
Unmasked-calculated*	7.61	9.83	7.81

*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 7.61 differs from the reported value 3.53 by more than 10 %

9 Map-model fit [i](#)

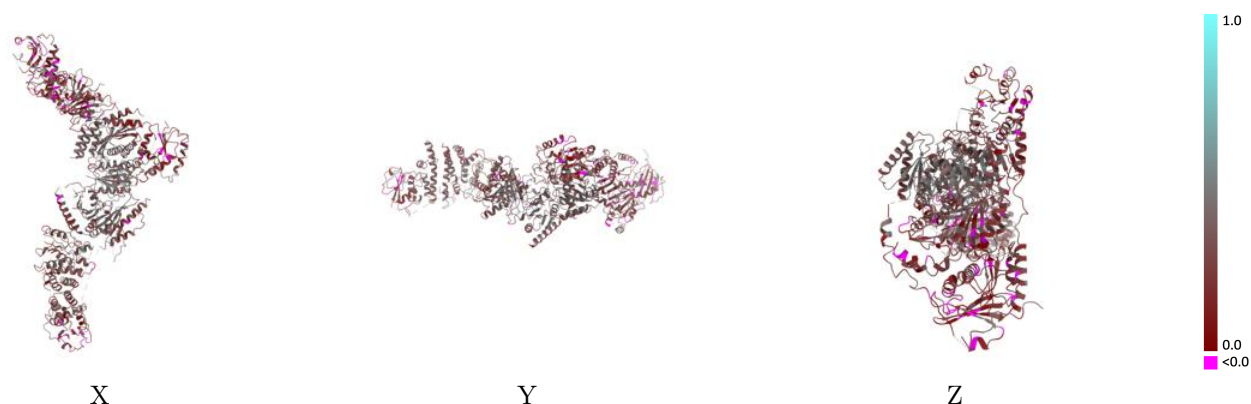
This section contains information regarding the fit between EMDB map EMD-27435 and PDB model 8DHB. Per-residue inclusion information can be found in section [3](#) on page [16](#).

9.1 Map-model overlay [i](#)



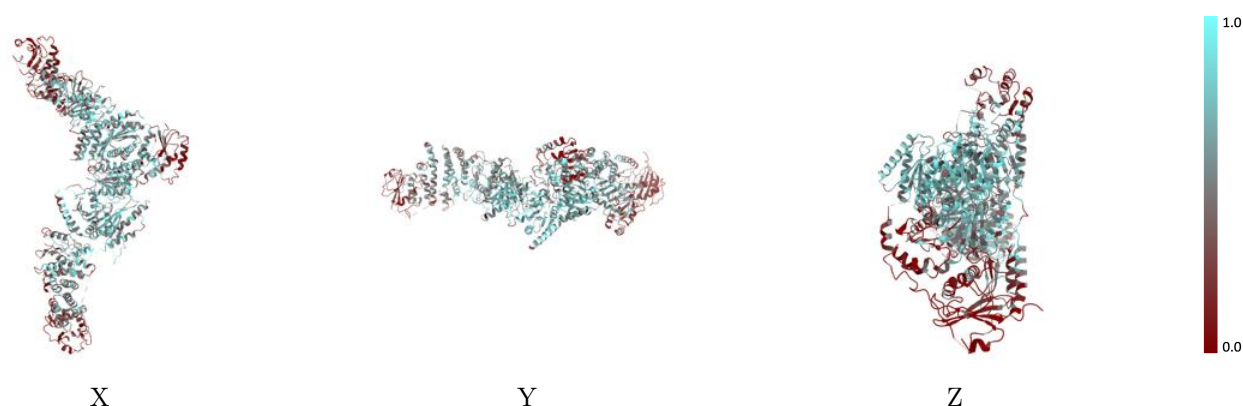
The images above show the 3D surface view of the map at the recommended contour level 0.48 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



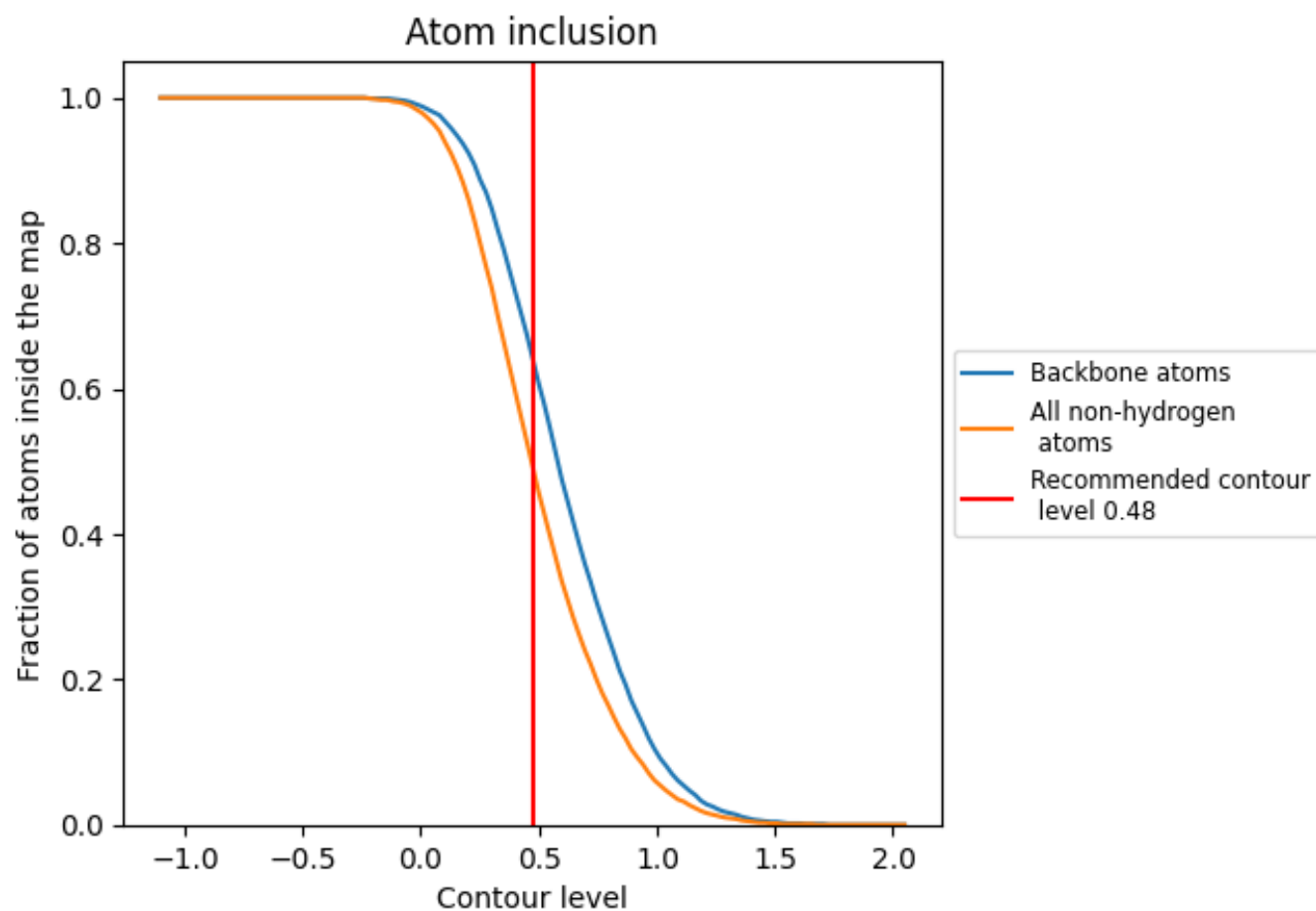
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.48).

9.4 Atom inclusion [i](#)



At the recommended contour level, 63% of all backbone atoms, 48% 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 (0.48) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4850	0.2970
A	0.6850	0.3890
B	0.4720	0.2600
C	0.3100	0.2750
D	0.5640	0.2210
E	0.3180	0.2220
F	0.0750	0.1780
G	0.3590	0.2140
H	0.4310	0.3270
I	0.5480	0.3290
J	0.4560	0.3060

1.0

0.0

<0.0