wwPDB EM Validation Summary Report

Dec 2, 2024 – 11:37 AM EST

PDB ID	:	8TLD
EMDB ID	:	EMD-41367
Title	:	Structure of the IL-5 Signaling Complex
Authors	:	Caveney, N.A.; Garcia, K.C.
Deposited on	:	2023-07-26
Resolution	:	3.60 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

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

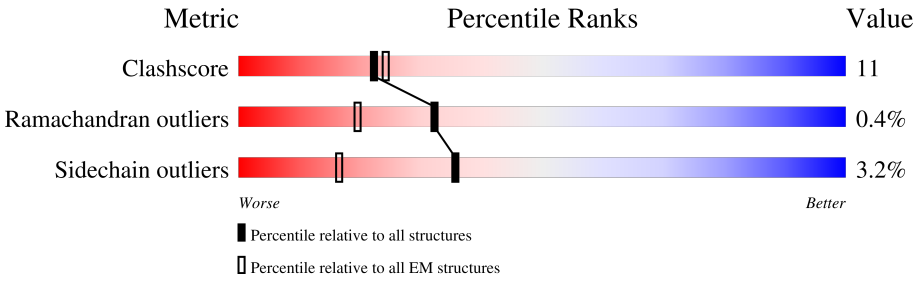
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

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 3.60 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	B	717	11% · 87%
1	E	717	12% · 84%
2	C	146	10% 47% 26% · 27%
2	D	146	13% 43% 28% · 25%
3	F	392	60% 18% · 21%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 5982 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 Cytokine receptor common subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	94	Total	C	N	O	S	0	0
			758	473	134	143	8		
1	E	113	Total	C	N	O	S	0	0
			942	585	174	179	4		

There are 594 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-234	ASP	-	expression tag	UNP P32927
B	-233	TYR	-	expression tag	UNP P32927
B	-232	LYS	-	expression tag	UNP P32927
B	-231	ASP	-	expression tag	UNP P32927
B	-230	ASP	-	expression tag	UNP P32927
B	-229	ASP	-	expression tag	UNP P32927
B	-228	ASP	-	expression tag	UNP P32927
B	-227	LYS	-	expression tag	UNP P32927
B	-226	MET	-	expression tag	UNP P32927
B	-225	VAL	-	expression tag	UNP P32927
B	-224	SER	-	expression tag	UNP P32927
B	-223	LYS	-	expression tag	UNP P32927
B	-222	GLY	-	expression tag	UNP P32927
B	-221	GLU	-	expression tag	UNP P32927
B	-220	GLU	-	expression tag	UNP P32927
B	-219	LEU	-	expression tag	UNP P32927
B	-218	PHE	-	expression tag	UNP P32927
B	-217	THR	-	expression tag	UNP P32927
B	-216	GLY	-	expression tag	UNP P32927
B	-215	VAL	-	expression tag	UNP P32927
B	-214	VAL	-	expression tag	UNP P32927
B	-213	PRO	-	expression tag	UNP P32927
B	-212	ILE	-	expression tag	UNP P32927
B	-211	LEU	-	expression tag	UNP P32927
B	-210	VAL	-	expression tag	UNP P32927
B	-209	GLU	-	expression tag	UNP P32927

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-208	LEU	-	expression tag	UNP P32927
B	-207	ASP	-	expression tag	UNP P32927
B	-206	GLY	-	expression tag	UNP P32927
B	-205	ASP	-	expression tag	UNP P32927
B	-204	VAL	-	expression tag	UNP P32927
B	-203	ASN	-	expression tag	UNP P32927
B	-202	GLY	-	expression tag	UNP P32927
B	-201	HIS	-	expression tag	UNP P32927
B	-200	LYS	-	expression tag	UNP P32927
B	-199	PHE	-	expression tag	UNP P32927
B	-198	SER	-	expression tag	UNP P32927
B	-197	VAL	-	expression tag	UNP P32927
B	-196	SER	-	expression tag	UNP P32927
B	-195	GLY	-	expression tag	UNP P32927
B	-194	GLU	-	expression tag	UNP P32927
B	-193	GLY	-	expression tag	UNP P32927
B	-192	GLU	-	expression tag	UNP P32927
B	-191	GLY	-	expression tag	UNP P32927
B	-190	ASP	-	expression tag	UNP P32927
B	-189	ALA	-	expression tag	UNP P32927
B	-188	THR	-	expression tag	UNP P32927
B	-187	TYR	-	expression tag	UNP P32927
B	-186	GLY	-	expression tag	UNP P32927
B	-185	LYS	-	expression tag	UNP P32927
B	-184	LEU	-	expression tag	UNP P32927
B	-183	THR	-	expression tag	UNP P32927
B	-182	LEU	-	expression tag	UNP P32927
B	-181	LYS	-	expression tag	UNP P32927
B	-180	PHE	-	expression tag	UNP P32927
B	-179	ILE	-	expression tag	UNP P32927
B	-178	CYS	-	expression tag	UNP P32927
B	-177	THR	-	expression tag	UNP P32927
B	-176	THR	-	expression tag	UNP P32927
B	-175	GLY	-	expression tag	UNP P32927
B	-174	LYS	-	expression tag	UNP P32927
B	-173	LEU	-	expression tag	UNP P32927
B	-172	PRO	-	expression tag	UNP P32927
B	-171	VAL	-	expression tag	UNP P32927
B	-170	PRO	-	expression tag	UNP P32927
B	-169	TRP	-	expression tag	UNP P32927
B	-168	PRO	-	expression tag	UNP P32927
B	-167	THR	-	expression tag	UNP P32927

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-166	LEU	-	expression tag	UNP P32927
B	-165	VAL	-	expression tag	UNP P32927
B	-164	THR	-	expression tag	UNP P32927
B	-163	THR	-	expression tag	UNP P32927
B	-162	LEU	-	expression tag	UNP P32927
B	-161	THR	-	expression tag	UNP P32927
B	-160	TYR	-	expression tag	UNP P32927
B	-159	GLY	-	expression tag	UNP P32927
B	-158	VAL	-	expression tag	UNP P32927
B	-157	GLN	-	expression tag	UNP P32927
B	-156	CYS	-	expression tag	UNP P32927
B	-155	PHE	-	expression tag	UNP P32927
B	-154	SER	-	expression tag	UNP P32927
B	-153	ARG	-	expression tag	UNP P32927
B	-152	TYR	-	expression tag	UNP P32927
B	-151	PRO	-	expression tag	UNP P32927
B	-150	ASP	-	expression tag	UNP P32927
B	-149	HIS	-	expression tag	UNP P32927
B	-148	MET	-	expression tag	UNP P32927
B	-147	LYS	-	expression tag	UNP P32927
B	-146	GLN	-	expression tag	UNP P32927
B	-145	HIS	-	expression tag	UNP P32927
B	-144	ASP	-	expression tag	UNP P32927
B	-143	PHE	-	expression tag	UNP P32927
B	-142	PHE	-	expression tag	UNP P32927
B	-141	LYS	-	expression tag	UNP P32927
B	-140	SER	-	expression tag	UNP P32927
B	-139	ALA	-	expression tag	UNP P32927
B	-138	MET	-	expression tag	UNP P32927
B	-137	PRO	-	expression tag	UNP P32927
B	-136	GLU	-	expression tag	UNP P32927
B	-135	GLY	-	expression tag	UNP P32927
B	-134	TYR	-	expression tag	UNP P32927
B	-133	VAL	-	expression tag	UNP P32927
B	-132	GLN	-	expression tag	UNP P32927
B	-131	GLU	-	expression tag	UNP P32927
B	-130	ARG	-	expression tag	UNP P32927
B	-129	THR	-	expression tag	UNP P32927
B	-128	ILE	-	expression tag	UNP P32927
B	-127	PHE	-	expression tag	UNP P32927
B	-126	PHE	-	expression tag	UNP P32927
B	-125	LYS	-	expression tag	UNP P32927

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-124	ASP	-	expression tag	UNP P32927
B	-123	ASP	-	expression tag	UNP P32927
B	-122	GLY	-	expression tag	UNP P32927
B	-121	ASN	-	expression tag	UNP P32927
B	-120	TYR	-	expression tag	UNP P32927
B	-119	LYS	-	expression tag	UNP P32927
B	-118	THR	-	expression tag	UNP P32927
B	-117	ARG	-	expression tag	UNP P32927
B	-116	ALA	-	expression tag	UNP P32927
B	-115	GLU	-	expression tag	UNP P32927
B	-114	VAL	-	expression tag	UNP P32927
B	-113	LYS	-	expression tag	UNP P32927
B	-112	PHE	-	expression tag	UNP P32927
B	-111	GLU	-	expression tag	UNP P32927
B	-110	GLY	-	expression tag	UNP P32927
B	-109	ASP	-	expression tag	UNP P32927
B	-108	THR	-	expression tag	UNP P32927
B	-107	LEU	-	expression tag	UNP P32927
B	-106	VAL	-	expression tag	UNP P32927
B	-105	ASN	-	expression tag	UNP P32927
B	-104	ARG	-	expression tag	UNP P32927
B	-103	ILE	-	expression tag	UNP P32927
B	-102	GLU	-	expression tag	UNP P32927
B	-101	LEU	-	expression tag	UNP P32927
B	-100	LYS	-	expression tag	UNP P32927
B	-99	GLY	-	expression tag	UNP P32927
B	-98	ILE	-	expression tag	UNP P32927
B	-97	ASP	-	expression tag	UNP P32927
B	-96	PHE	-	expression tag	UNP P32927
B	-95	LYS	-	expression tag	UNP P32927
B	-94	GLU	-	expression tag	UNP P32927
B	-93	ASP	-	expression tag	UNP P32927
B	-92	GLY	-	expression tag	UNP P32927
B	-91	ASN	-	expression tag	UNP P32927
B	-90	ILE	-	expression tag	UNP P32927
B	-89	LEU	-	expression tag	UNP P32927
B	-88	GLY	-	expression tag	UNP P32927
B	-87	HIS	-	expression tag	UNP P32927
B	-86	LYS	-	expression tag	UNP P32927
B	-85	LEU	-	expression tag	UNP P32927
B	-84	GLU	-	expression tag	UNP P32927
B	-83	TYR	-	expression tag	UNP P32927

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-82	ASN	-	expression tag	UNP P32927
B	-81	TYR	-	expression tag	UNP P32927
B	-80	ASN	-	expression tag	UNP P32927
B	-79	SER	-	expression tag	UNP P32927
B	-78	HIS	-	expression tag	UNP P32927
B	-77	ASN	-	expression tag	UNP P32927
B	-76	VAL	-	expression tag	UNP P32927
B	-75	TYR	-	expression tag	UNP P32927
B	-74	ILE	-	expression tag	UNP P32927
B	-73	MET	-	expression tag	UNP P32927
B	-72	ALA	-	expression tag	UNP P32927
B	-71	ASP	-	expression tag	UNP P32927
B	-70	LYS	-	expression tag	UNP P32927
B	-69	GLN	-	expression tag	UNP P32927
B	-68	LYS	-	expression tag	UNP P32927
B	-67	ASN	-	expression tag	UNP P32927
B	-66	GLY	-	expression tag	UNP P32927
B	-65	ILE	-	expression tag	UNP P32927
B	-64	LYS	-	expression tag	UNP P32927
B	-63	VAL	-	expression tag	UNP P32927
B	-62	ASN	-	expression tag	UNP P32927
B	-61	PHE	-	expression tag	UNP P32927
B	-60	LYS	-	expression tag	UNP P32927
B	-59	ILE	-	expression tag	UNP P32927
B	-58	ARG	-	expression tag	UNP P32927
B	-57	HIS	-	expression tag	UNP P32927
B	-56	ASN	-	expression tag	UNP P32927
B	-55	ILE	-	expression tag	UNP P32927
B	-54	GLU	-	expression tag	UNP P32927
B	-53	ASP	-	expression tag	UNP P32927
B	-52	GLY	-	expression tag	UNP P32927
B	-51	SER	-	expression tag	UNP P32927
B	-50	VAL	-	expression tag	UNP P32927
B	-49	GLN	-	expression tag	UNP P32927
B	-48	LEU	-	expression tag	UNP P32927
B	-47	ALA	-	expression tag	UNP P32927
B	-46	ASP	-	expression tag	UNP P32927
B	-45	HIS	-	expression tag	UNP P32927
B	-44	TYR	-	expression tag	UNP P32927
B	-43	GLN	-	expression tag	UNP P32927
B	-42	GLN	-	expression tag	UNP P32927
B	-41	ASN	-	expression tag	UNP P32927

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-40	THR	-	expression tag	UNP P32927
B	-39	PRO	-	expression tag	UNP P32927
B	-38	ILE	-	expression tag	UNP P32927
B	-37	GLY	-	expression tag	UNP P32927
B	-36	ASP	-	expression tag	UNP P32927
B	-35	GLY	-	expression tag	UNP P32927
B	-34	PRO	-	expression tag	UNP P32927
B	-33	VAL	-	expression tag	UNP P32927
B	-32	LEU	-	expression tag	UNP P32927
B	-31	LEU	-	expression tag	UNP P32927
B	-30	PRO	-	expression tag	UNP P32927
B	-29	ASP	-	expression tag	UNP P32927
B	-28	ASN	-	expression tag	UNP P32927
B	-27	HIS	-	expression tag	UNP P32927
B	-26	TYR	-	expression tag	UNP P32927
B	-25	LEU	-	expression tag	UNP P32927
B	-24	SER	-	expression tag	UNP P32927
B	-23	THR	-	expression tag	UNP P32927
B	-22	GLN	-	expression tag	UNP P32927
B	-21	SER	-	expression tag	UNP P32927
B	-20	ALA	-	expression tag	UNP P32927
B	-19	LEU	-	expression tag	UNP P32927
B	-18	SER	-	expression tag	UNP P32927
B	-17	LYS	-	expression tag	UNP P32927
B	-16	ASP	-	expression tag	UNP P32927
B	-15	PRO	-	expression tag	UNP P32927
B	-14	ASN	-	expression tag	UNP P32927
B	-13	GLU	-	expression tag	UNP P32927
B	-12	LYS	-	expression tag	UNP P32927
B	-11	ARG	-	expression tag	UNP P32927
B	-10	ASP	-	expression tag	UNP P32927
B	-9	HIS	-	expression tag	UNP P32927
B	-8	MET	-	expression tag	UNP P32927
B	-7	VAL	-	expression tag	UNP P32927
B	-6	LEU	-	expression tag	UNP P32927
B	-5	LEU	-	expression tag	UNP P32927
B	-4	GLU	-	expression tag	UNP P32927
B	-3	PHE	-	expression tag	UNP P32927
B	-2	VAL	-	expression tag	UNP P32927
B	-1	THR	-	expression tag	UNP P32927
B	0	ALA	-	expression tag	UNP P32927
B	1	ALA	-	expression tag	UNP P32927

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Chain	Residue	Modelled	Actual	Comment	Reference
B	2	GLY	-	expression tag	UNP P32927
B	3	ILE	-	expression tag	UNP P32927
B	4	THR	-	expression tag	UNP P32927
B	5	LEU	-	expression tag	UNP P32927
B	6	GLY	-	expression tag	UNP P32927
B	7	MET	-	expression tag	UNP P32927
B	8	ASP	-	expression tag	UNP P32927
B	9	GLU	-	expression tag	UNP P32927
B	10	LEU	-	expression tag	UNP P32927
B	11	TYR	-	expression tag	UNP P32927
B	12	LYS	-	expression tag	UNP P32927
B	13	LEU	-	expression tag	UNP P32927
B	14	GLU	-	expression tag	UNP P32927
B	15	VAL	-	expression tag	UNP P32927
B	16	LEU	-	expression tag	UNP P32927
B	17	PHE	-	expression tag	UNP P32927
B	18	GLN	-	expression tag	UNP P32927
B	19	GLY	-	expression tag	UNP P32927
B	20	PRO	-	expression tag	UNP P32927
B	21	GLY	-	expression tag	UNP P32927
B	22	SER	-	expression tag	UNP P32927
B	440	GLY	-	expression tag	UNP P32927
B	441	GLY	-	expression tag	UNP P32927
B	442	GLY	-	expression tag	UNP P32927
B	443	GLY	-	expression tag	UNP P32927
B	444	SER	-	expression tag	UNP P32927
B	445	THR	-	expression tag	UNP P32927
B	446	THR	-	expression tag	UNP P32927
B	447	ALA	-	expression tag	UNP P32927
B	448	PRO	-	expression tag	UNP P32927
B	449	SER	-	expression tag	UNP P32927
B	450	ALA	-	expression tag	UNP P32927
B	451	GLN	-	expression tag	UNP P32927
B	452	LEU	-	expression tag	UNP P32927
B	453	GLU	-	expression tag	UNP P32927
B	454	LYS	-	expression tag	UNP P32927
B	455	GLU	-	expression tag	UNP P32927
B	456	LEU	-	expression tag	UNP P32927
B	457	GLN	-	expression tag	UNP P32927
B	458	ALA	-	expression tag	UNP P32927
B	459	LEU	-	expression tag	UNP P32927
B	460	GLU	-	expression tag	UNP P32927

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Chain	Residue	Modelled	Actual	Comment	Reference
B	461	LYS	-	expression tag	UNP P32927
B	462	GLU	-	expression tag	UNP P32927
B	463	ASN	-	expression tag	UNP P32927
B	464	ALA	-	expression tag	UNP P32927
B	465	GLN	-	expression tag	UNP P32927
B	466	LEU	-	expression tag	UNP P32927
B	467	GLU	-	expression tag	UNP P32927
B	468	TRP	-	expression tag	UNP P32927
B	469	GLU	-	expression tag	UNP P32927
B	470	LEU	-	expression tag	UNP P32927
B	471	GLN	-	expression tag	UNP P32927
B	472	ALA	-	expression tag	UNP P32927
B	473	LEU	-	expression tag	UNP P32927
B	474	GLU	-	expression tag	UNP P32927
B	475	LYS	-	expression tag	UNP P32927
B	476	GLU	-	expression tag	UNP P32927
B	477	LEU	-	expression tag	UNP P32927
B	478	ALA	-	expression tag	UNP P32927
B	479	GLN	-	expression tag	UNP P32927
E	-234	ASP	-	expression tag	UNP P32927
E	-233	TYR	-	expression tag	UNP P32927
E	-232	LYS	-	expression tag	UNP P32927
E	-231	ASP	-	expression tag	UNP P32927
E	-230	ASP	-	expression tag	UNP P32927
E	-229	ASP	-	expression tag	UNP P32927
E	-228	ASP	-	expression tag	UNP P32927
E	-227	LYS	-	expression tag	UNP P32927
E	-226	MET	-	expression tag	UNP P32927
E	-225	VAL	-	expression tag	UNP P32927
E	-224	SER	-	expression tag	UNP P32927
E	-223	LYS	-	expression tag	UNP P32927
E	-222	GLY	-	expression tag	UNP P32927
E	-221	GLU	-	expression tag	UNP P32927
E	-220	GLU	-	expression tag	UNP P32927
E	-219	LEU	-	expression tag	UNP P32927
E	-218	PHE	-	expression tag	UNP P32927
E	-217	THR	-	expression tag	UNP P32927
E	-216	GLY	-	expression tag	UNP P32927
E	-215	VAL	-	expression tag	UNP P32927
E	-214	VAL	-	expression tag	UNP P32927
E	-213	PRO	-	expression tag	UNP P32927
E	-212	ILE	-	expression tag	UNP P32927

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-211	LEU	-	expression tag	UNP P32927
E	-210	VAL	-	expression tag	UNP P32927
E	-209	GLU	-	expression tag	UNP P32927
E	-208	LEU	-	expression tag	UNP P32927
E	-207	ASP	-	expression tag	UNP P32927
E	-206	GLY	-	expression tag	UNP P32927
E	-205	ASP	-	expression tag	UNP P32927
E	-204	VAL	-	expression tag	UNP P32927
E	-203	ASN	-	expression tag	UNP P32927
E	-202	GLY	-	expression tag	UNP P32927
E	-201	HIS	-	expression tag	UNP P32927
E	-200	LYS	-	expression tag	UNP P32927
E	-199	PHE	-	expression tag	UNP P32927
E	-198	SER	-	expression tag	UNP P32927
E	-197	VAL	-	expression tag	UNP P32927
E	-196	SER	-	expression tag	UNP P32927
E	-195	GLY	-	expression tag	UNP P32927
E	-194	GLU	-	expression tag	UNP P32927
E	-193	GLY	-	expression tag	UNP P32927
E	-192	GLU	-	expression tag	UNP P32927
E	-191	GLY	-	expression tag	UNP P32927
E	-190	ASP	-	expression tag	UNP P32927
E	-189	ALA	-	expression tag	UNP P32927
E	-188	THR	-	expression tag	UNP P32927
E	-187	TYR	-	expression tag	UNP P32927
E	-186	GLY	-	expression tag	UNP P32927
E	-185	LYS	-	expression tag	UNP P32927
E	-184	LEU	-	expression tag	UNP P32927
E	-183	THR	-	expression tag	UNP P32927
E	-182	LEU	-	expression tag	UNP P32927
E	-181	LYS	-	expression tag	UNP P32927
E	-180	PHE	-	expression tag	UNP P32927
E	-179	ILE	-	expression tag	UNP P32927
E	-178	CYS	-	expression tag	UNP P32927
E	-177	THR	-	expression tag	UNP P32927
E	-176	THR	-	expression tag	UNP P32927
E	-175	GLY	-	expression tag	UNP P32927
E	-174	LYS	-	expression tag	UNP P32927
E	-173	LEU	-	expression tag	UNP P32927
E	-172	PRO	-	expression tag	UNP P32927
E	-171	VAL	-	expression tag	UNP P32927
E	-170	PRO	-	expression tag	UNP P32927

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-169	TRP	-	expression tag	UNP P32927
E	-168	PRO	-	expression tag	UNP P32927
E	-167	THR	-	expression tag	UNP P32927
E	-166	LEU	-	expression tag	UNP P32927
E	-165	VAL	-	expression tag	UNP P32927
E	-164	THR	-	expression tag	UNP P32927
E	-163	THR	-	expression tag	UNP P32927
E	-162	LEU	-	expression tag	UNP P32927
E	-161	THR	-	expression tag	UNP P32927
E	-160	TYR	-	expression tag	UNP P32927
E	-159	GLY	-	expression tag	UNP P32927
E	-158	VAL	-	expression tag	UNP P32927
E	-157	GLN	-	expression tag	UNP P32927
E	-156	CYS	-	expression tag	UNP P32927
E	-155	PHE	-	expression tag	UNP P32927
E	-154	SER	-	expression tag	UNP P32927
E	-153	ARG	-	expression tag	UNP P32927
E	-152	TYR	-	expression tag	UNP P32927
E	-151	PRO	-	expression tag	UNP P32927
E	-150	ASP	-	expression tag	UNP P32927
E	-149	HIS	-	expression tag	UNP P32927
E	-148	MET	-	expression tag	UNP P32927
E	-147	LYS	-	expression tag	UNP P32927
E	-146	GLN	-	expression tag	UNP P32927
E	-145	HIS	-	expression tag	UNP P32927
E	-144	ASP	-	expression tag	UNP P32927
E	-143	PHE	-	expression tag	UNP P32927
E	-142	PHE	-	expression tag	UNP P32927
E	-141	LYS	-	expression tag	UNP P32927
E	-140	SER	-	expression tag	UNP P32927
E	-139	ALA	-	expression tag	UNP P32927
E	-138	MET	-	expression tag	UNP P32927
E	-137	PRO	-	expression tag	UNP P32927
E	-136	GLU	-	expression tag	UNP P32927
E	-135	GLY	-	expression tag	UNP P32927
E	-134	TYR	-	expression tag	UNP P32927
E	-133	VAL	-	expression tag	UNP P32927
E	-132	GLN	-	expression tag	UNP P32927
E	-131	GLU	-	expression tag	UNP P32927
E	-130	ARG	-	expression tag	UNP P32927
E	-129	THR	-	expression tag	UNP P32927
E	-128	ILE	-	expression tag	UNP P32927

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-127	PHE	-	expression tag	UNP P32927
E	-126	PHE	-	expression tag	UNP P32927
E	-125	LYS	-	expression tag	UNP P32927
E	-124	ASP	-	expression tag	UNP P32927
E	-123	ASP	-	expression tag	UNP P32927
E	-122	GLY	-	expression tag	UNP P32927
E	-121	ASN	-	expression tag	UNP P32927
E	-120	TYR	-	expression tag	UNP P32927
E	-119	LYS	-	expression tag	UNP P32927
E	-118	THR	-	expression tag	UNP P32927
E	-117	ARG	-	expression tag	UNP P32927
E	-116	ALA	-	expression tag	UNP P32927
E	-115	GLU	-	expression tag	UNP P32927
E	-114	VAL	-	expression tag	UNP P32927
E	-113	LYS	-	expression tag	UNP P32927
E	-112	PHE	-	expression tag	UNP P32927
E	-111	GLU	-	expression tag	UNP P32927
E	-110	GLY	-	expression tag	UNP P32927
E	-109	ASP	-	expression tag	UNP P32927
E	-108	THR	-	expression tag	UNP P32927
E	-107	LEU	-	expression tag	UNP P32927
E	-106	VAL	-	expression tag	UNP P32927
E	-105	ASN	-	expression tag	UNP P32927
E	-104	ARG	-	expression tag	UNP P32927
E	-103	ILE	-	expression tag	UNP P32927
E	-102	GLU	-	expression tag	UNP P32927
E	-101	LEU	-	expression tag	UNP P32927
E	-100	LYS	-	expression tag	UNP P32927
E	-99	GLY	-	expression tag	UNP P32927
E	-98	ILE	-	expression tag	UNP P32927
E	-97	ASP	-	expression tag	UNP P32927
E	-96	PHE	-	expression tag	UNP P32927
E	-95	LYS	-	expression tag	UNP P32927
E	-94	GLU	-	expression tag	UNP P32927
E	-93	ASP	-	expression tag	UNP P32927
E	-92	GLY	-	expression tag	UNP P32927
E	-91	ASN	-	expression tag	UNP P32927
E	-90	ILE	-	expression tag	UNP P32927
E	-89	LEU	-	expression tag	UNP P32927
E	-88	GLY	-	expression tag	UNP P32927
E	-87	HIS	-	expression tag	UNP P32927
E	-86	LYS	-	expression tag	UNP P32927

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-85	LEU	-	expression tag	UNP P32927
E	-84	GLU	-	expression tag	UNP P32927
E	-83	TYR	-	expression tag	UNP P32927
E	-82	ASN	-	expression tag	UNP P32927
E	-81	TYR	-	expression tag	UNP P32927
E	-80	ASN	-	expression tag	UNP P32927
E	-79	SER	-	expression tag	UNP P32927
E	-78	HIS	-	expression tag	UNP P32927
E	-77	ASN	-	expression tag	UNP P32927
E	-76	VAL	-	expression tag	UNP P32927
E	-75	TYR	-	expression tag	UNP P32927
E	-74	ILE	-	expression tag	UNP P32927
E	-73	MET	-	expression tag	UNP P32927
E	-72	ALA	-	expression tag	UNP P32927
E	-71	ASP	-	expression tag	UNP P32927
E	-70	LYS	-	expression tag	UNP P32927
E	-69	GLN	-	expression tag	UNP P32927
E	-68	LYS	-	expression tag	UNP P32927
E	-67	ASN	-	expression tag	UNP P32927
E	-66	GLY	-	expression tag	UNP P32927
E	-65	ILE	-	expression tag	UNP P32927
E	-64	LYS	-	expression tag	UNP P32927
E	-63	VAL	-	expression tag	UNP P32927
E	-62	ASN	-	expression tag	UNP P32927
E	-61	PHE	-	expression tag	UNP P32927
E	-60	LYS	-	expression tag	UNP P32927
E	-59	ILE	-	expression tag	UNP P32927
E	-58	ARG	-	expression tag	UNP P32927
E	-57	HIS	-	expression tag	UNP P32927
E	-56	ASN	-	expression tag	UNP P32927
E	-55	ILE	-	expression tag	UNP P32927
E	-54	GLU	-	expression tag	UNP P32927
E	-53	ASP	-	expression tag	UNP P32927
E	-52	GLY	-	expression tag	UNP P32927
E	-51	SER	-	expression tag	UNP P32927
E	-50	VAL	-	expression tag	UNP P32927
E	-49	GLN	-	expression tag	UNP P32927
E	-48	LEU	-	expression tag	UNP P32927
E	-47	ALA	-	expression tag	UNP P32927
E	-46	ASP	-	expression tag	UNP P32927
E	-45	HIS	-	expression tag	UNP P32927
E	-44	TYR	-	expression tag	UNP P32927

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-43	GLN	-	expression tag	UNP P32927
E	-42	GLN	-	expression tag	UNP P32927
E	-41	ASN	-	expression tag	UNP P32927
E	-40	THR	-	expression tag	UNP P32927
E	-39	PRO	-	expression tag	UNP P32927
E	-38	ILE	-	expression tag	UNP P32927
E	-37	GLY	-	expression tag	UNP P32927
E	-36	ASP	-	expression tag	UNP P32927
E	-35	GLY	-	expression tag	UNP P32927
E	-34	PRO	-	expression tag	UNP P32927
E	-33	VAL	-	expression tag	UNP P32927
E	-32	LEU	-	expression tag	UNP P32927
E	-31	LEU	-	expression tag	UNP P32927
E	-30	PRO	-	expression tag	UNP P32927
E	-29	ASP	-	expression tag	UNP P32927
E	-28	ASN	-	expression tag	UNP P32927
E	-27	HIS	-	expression tag	UNP P32927
E	-26	TYR	-	expression tag	UNP P32927
E	-25	LEU	-	expression tag	UNP P32927
E	-24	SER	-	expression tag	UNP P32927
E	-23	THR	-	expression tag	UNP P32927
E	-22	GLN	-	expression tag	UNP P32927
E	-21	SER	-	expression tag	UNP P32927
E	-20	ALA	-	expression tag	UNP P32927
E	-19	LEU	-	expression tag	UNP P32927
E	-18	SER	-	expression tag	UNP P32927
E	-17	LYS	-	expression tag	UNP P32927
E	-16	ASP	-	expression tag	UNP P32927
E	-15	PRO	-	expression tag	UNP P32927
E	-14	ASN	-	expression tag	UNP P32927
E	-13	GLU	-	expression tag	UNP P32927
E	-12	LYS	-	expression tag	UNP P32927
E	-11	ARG	-	expression tag	UNP P32927
E	-10	ASP	-	expression tag	UNP P32927
E	-9	HIS	-	expression tag	UNP P32927
E	-8	MET	-	expression tag	UNP P32927
E	-7	VAL	-	expression tag	UNP P32927
E	-6	LEU	-	expression tag	UNP P32927
E	-5	LEU	-	expression tag	UNP P32927
E	-4	GLU	-	expression tag	UNP P32927
E	-3	PHE	-	expression tag	UNP P32927
E	-2	VAL	-	expression tag	UNP P32927

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-1	THR	-	expression tag	UNP P32927
E	0	ALA	-	expression tag	UNP P32927
E	1	ALA	-	expression tag	UNP P32927
E	2	GLY	-	expression tag	UNP P32927
E	3	ILE	-	expression tag	UNP P32927
E	4	THR	-	expression tag	UNP P32927
E	5	LEU	-	expression tag	UNP P32927
E	6	GLY	-	expression tag	UNP P32927
E	7	MET	-	expression tag	UNP P32927
E	8	ASP	-	expression tag	UNP P32927
E	9	GLU	-	expression tag	UNP P32927
E	10	LEU	-	expression tag	UNP P32927
E	11	TYR	-	expression tag	UNP P32927
E	12	LYS	-	expression tag	UNP P32927
E	13	LEU	-	expression tag	UNP P32927
E	14	GLU	-	expression tag	UNP P32927
E	15	VAL	-	expression tag	UNP P32927
E	16	LEU	-	expression tag	UNP P32927
E	17	PHE	-	expression tag	UNP P32927
E	18	GLN	-	expression tag	UNP P32927
E	19	GLY	-	expression tag	UNP P32927
E	20	PRO	-	expression tag	UNP P32927
E	21	GLY	-	expression tag	UNP P32927
E	22	SER	-	expression tag	UNP P32927
E	443	GLY	-	expression tag	UNP P32927
E	444	GLY	-	expression tag	UNP P32927
E	445	GLY	-	expression tag	UNP P32927
E	446	GLY	-	expression tag	UNP P32927
E	447	SER	-	expression tag	UNP P32927
E	448	THR	-	expression tag	UNP P32927
E	449	THR	-	expression tag	UNP P32927
E	450	ALA	-	expression tag	UNP P32927
E	451	PRO	-	expression tag	UNP P32927
E	452	SER	-	expression tag	UNP P32927
E	453	ALA	-	expression tag	UNP P32927
E	454	GLN	-	expression tag	UNP P32927
E	455	LEU	-	expression tag	UNP P32927
E	456	GLU	-	expression tag	UNP P32927
E	457	LYS	-	expression tag	UNP P32927
E	458	GLU	-	expression tag	UNP P32927
E	459	LEU	-	expression tag	UNP P32927
E	460	GLN	-	expression tag	UNP P32927

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Chain	Residue	Modelled	Actual	Comment	Reference
E	461	ALA	-	expression tag	UNP P32927
E	462	LEU	-	expression tag	UNP P32927
E	463	GLU	-	expression tag	UNP P32927
E	464	LYS	-	expression tag	UNP P32927
E	465	GLU	-	expression tag	UNP P32927
E	466	ASN	-	expression tag	UNP P32927
E	467	ALA	-	expression tag	UNP P32927
E	468	GLN	-	expression tag	UNP P32927
E	469	LEU	-	expression tag	UNP P32927
E	470	GLU	-	expression tag	UNP P32927
E	471	TRP	-	expression tag	UNP P32927
E	472	GLU	-	expression tag	UNP P32927
E	473	LEU	-	expression tag	UNP P32927
E	474	GLN	-	expression tag	UNP P32927
E	475	ALA	-	expression tag	UNP P32927
E	476	LEU	-	expression tag	UNP P32927
E	477	GLU	-	expression tag	UNP P32927
E	478	LYS	-	expression tag	UNP P32927
E	479	GLU	-	expression tag	UNP P32927
E	480	LEU	-	expression tag	UNP P32927
E	481	ALA	-	expression tag	UNP P32927
E	482	GLN	-	expression tag	UNP P32927

- Molecule 2 is a protein called Interleukin-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	107	Total	C	N	O	S	0	0
			862	548	152	159	3		
2	D	109	Total	C	N	O	S	0	0
			879	559	154	163	3		

There are 62 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	13	ASP	-	expression tag	UNP P05113
C	14	TYR	-	expression tag	UNP P05113
C	15	LYS	-	expression tag	UNP P05113
C	16	ASP	-	expression tag	UNP P05113
C	17	ASP	-	expression tag	UNP P05113
C	18	ASP	-	expression tag	UNP P05113
C	19	ASP	-	expression tag	UNP P05113
C	20	LYS	-	expression tag	UNP P05113

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Chain	Residue	Modelled	Actual	Comment	Reference
C	136	GLY	-	expression tag	UNP P05113
C	137	ALA	-	expression tag	UNP P05113
C	138	ALA	-	expression tag	UNP P05113
C	139	GLU	-	expression tag	UNP P05113
C	140	ASP	-	expression tag	UNP P05113
C	141	GLN	-	expression tag	UNP P05113
C	142	VAL	-	expression tag	UNP P05113
C	143	ASP	-	expression tag	UNP P05113
C	144	PRO	-	expression tag	UNP P05113
C	145	ARG	-	expression tag	UNP P05113
C	146	LEU	-	expression tag	UNP P05113
C	147	ILE	-	expression tag	UNP P05113
C	148	ASP	-	expression tag	UNP P05113
C	149	GLY	-	expression tag	UNP P05113
C	150	LYS	-	expression tag	UNP P05113
C	151	HIS	-	expression tag	UNP P05113
C	152	HIS	-	expression tag	UNP P05113
C	153	HIS	-	expression tag	UNP P05113
C	154	HIS	-	expression tag	UNP P05113
C	155	HIS	-	expression tag	UNP P05113
C	156	HIS	-	expression tag	UNP P05113
C	157	HIS	-	expression tag	UNP P05113
C	158	HIS	-	expression tag	UNP P05113
D	13	ASP	-	expression tag	UNP P05113
D	14	TYR	-	expression tag	UNP P05113
D	15	LYS	-	expression tag	UNP P05113
D	16	ASP	-	expression tag	UNP P05113
D	17	ASP	-	expression tag	UNP P05113
D	18	ASP	-	expression tag	UNP P05113
D	19	ASP	-	expression tag	UNP P05113
D	20	LYS	-	expression tag	UNP P05113
D	136	GLY	-	expression tag	UNP P05113
D	137	ALA	-	expression tag	UNP P05113
D	138	ALA	-	expression tag	UNP P05113
D	139	GLU	-	expression tag	UNP P05113
D	140	ASP	-	expression tag	UNP P05113
D	141	GLN	-	expression tag	UNP P05113
D	142	VAL	-	expression tag	UNP P05113
D	143	ASP	-	expression tag	UNP P05113
D	144	PRO	-	expression tag	UNP P05113
D	145	ARG	-	expression tag	UNP P05113
D	146	LEU	-	expression tag	UNP P05113

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Chain	Residue	Modelled	Actual	Comment	Reference
D	147	ILE	-	expression tag	UNP P05113
D	148	ASP	-	expression tag	UNP P05113
D	149	GLY	-	expression tag	UNP P05113
D	150	LYS	-	expression tag	UNP P05113
D	151	HIS	-	expression tag	UNP P05113
D	152	HIS	-	expression tag	UNP P05113
D	153	HIS	-	expression tag	UNP P05113
D	154	HIS	-	expression tag	UNP P05113
D	155	HIS	-	expression tag	UNP P05113
D	156	HIS	-	expression tag	UNP P05113
D	157	HIS	-	expression tag	UNP P05113
D	158	HIS	-	expression tag	UNP P05113

- Molecule 3 is a protein called Interleukin-5 receptor subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	308	Total	C	N	O	S	0	0
			2471	1571	421	470	9		

There are 71 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	13	ASP	-	expression tag	UNP Q01344
F	14	TYR	-	expression tag	UNP Q01344
F	15	LYS	-	expression tag	UNP Q01344
F	16	ASP	-	expression tag	UNP Q01344
F	17	ASP	-	expression tag	UNP Q01344
F	18	ASP	-	expression tag	UNP Q01344
F	19	ASP	-	expression tag	UNP Q01344
F	20	LYS	-	expression tag	UNP Q01344
F	342	GLY	-	expression tag	UNP Q01344
F	343	GLY	-	expression tag	UNP Q01344
F	344	GLY	-	expression tag	UNP Q01344
F	345	GLY	-	expression tag	UNP Q01344
F	346	SER	-	expression tag	UNP Q01344
F	347	THR	-	expression tag	UNP Q01344
F	348	THR	-	expression tag	UNP Q01344
F	349	ALA	-	expression tag	UNP Q01344
F	350	PRO	-	expression tag	UNP Q01344
F	351	SER	-	expression tag	UNP Q01344
F	352	ALA	-	expression tag	UNP Q01344
F	353	GLN	-	expression tag	UNP Q01344

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Chain	Residue	Modelled	Actual	Comment	Reference
F	354	LEU	-	expression tag	UNP Q01344
F	355	LYS	-	expression tag	UNP Q01344
F	356	LYS	-	expression tag	UNP Q01344
F	357	LYS	-	expression tag	UNP Q01344
F	358	LEU	-	expression tag	UNP Q01344
F	359	GLN	-	expression tag	UNP Q01344
F	360	ALA	-	expression tag	UNP Q01344
F	361	LEU	-	expression tag	UNP Q01344
F	362	LYS	-	expression tag	UNP Q01344
F	363	LYS	-	expression tag	UNP Q01344
F	364	LYS	-	expression tag	UNP Q01344
F	365	ASN	-	expression tag	UNP Q01344
F	366	ALA	-	expression tag	UNP Q01344
F	367	GLN	-	expression tag	UNP Q01344
F	368	LEU	-	expression tag	UNP Q01344
F	369	LYS	-	expression tag	UNP Q01344
F	370	TRP	-	expression tag	UNP Q01344
F	371	LYS	-	expression tag	UNP Q01344
F	372	LEU	-	expression tag	UNP Q01344
F	373	GLN	-	expression tag	UNP Q01344
F	374	ALA	-	expression tag	UNP Q01344
F	375	LEU	-	expression tag	UNP Q01344
F	376	LYS	-	expression tag	UNP Q01344
F	377	LYS	-	expression tag	UNP Q01344
F	378	LYS	-	expression tag	UNP Q01344
F	379	LEU	-	expression tag	UNP Q01344
F	380	ALA	-	expression tag	UNP Q01344
F	381	GLN	-	expression tag	UNP Q01344
F	382	GLY	-	expression tag	UNP Q01344
F	383	ALA	-	expression tag	UNP Q01344
F	384	ALA	-	expression tag	UNP Q01344
F	385	GLU	-	expression tag	UNP Q01344
F	386	ASP	-	expression tag	UNP Q01344
F	387	GLN	-	expression tag	UNP Q01344
F	388	VAL	-	expression tag	UNP Q01344
F	389	ASP	-	expression tag	UNP Q01344
F	390	PRO	-	expression tag	UNP Q01344
F	391	ARG	-	expression tag	UNP Q01344
F	392	LEU	-	expression tag	UNP Q01344
F	393	ILE	-	expression tag	UNP Q01344
F	394	ASP	-	expression tag	UNP Q01344
F	395	GLY	-	expression tag	UNP Q01344

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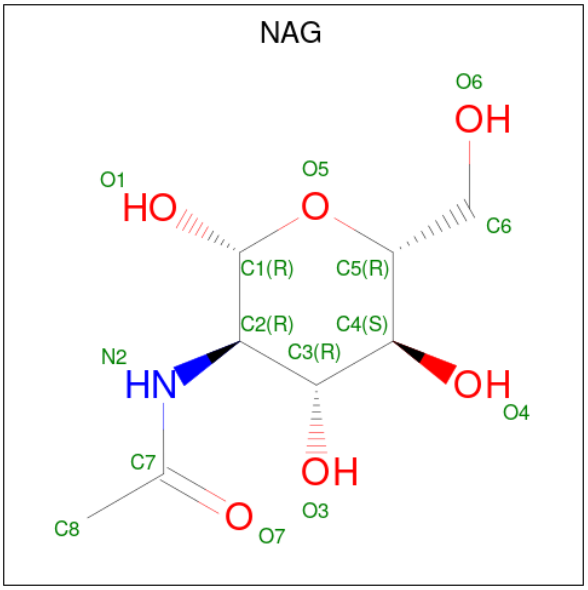
Chain	Residue	Modelled	Actual	Comment	Reference
F	396	LYS	-	expression tag	UNP Q01344
F	397	HIS	-	expression tag	UNP Q01344
F	398	HIS	-	expression tag	UNP Q01344
F	399	HIS	-	expression tag	UNP Q01344
F	400	HIS	-	expression tag	UNP Q01344
F	401	HIS	-	expression tag	UNP Q01344
F	402	HIS	-	expression tag	UNP Q01344
F	403	HIS	-	expression tag	UNP Q01344
F	404	HIS	-	expression tag	UNP Q01344

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



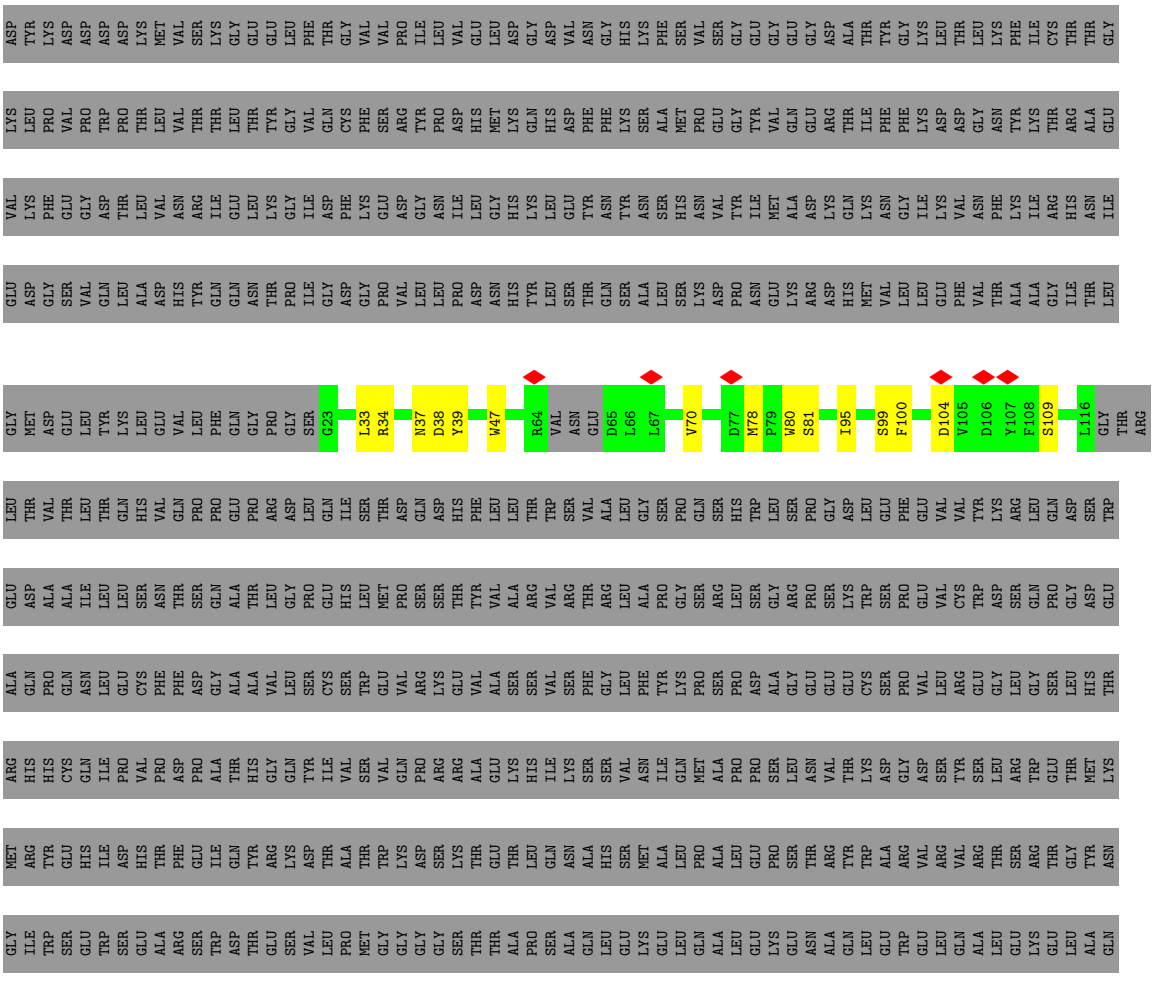
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	
4	F	1	Total	C	N	O	0
			14	8	1	5	

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.

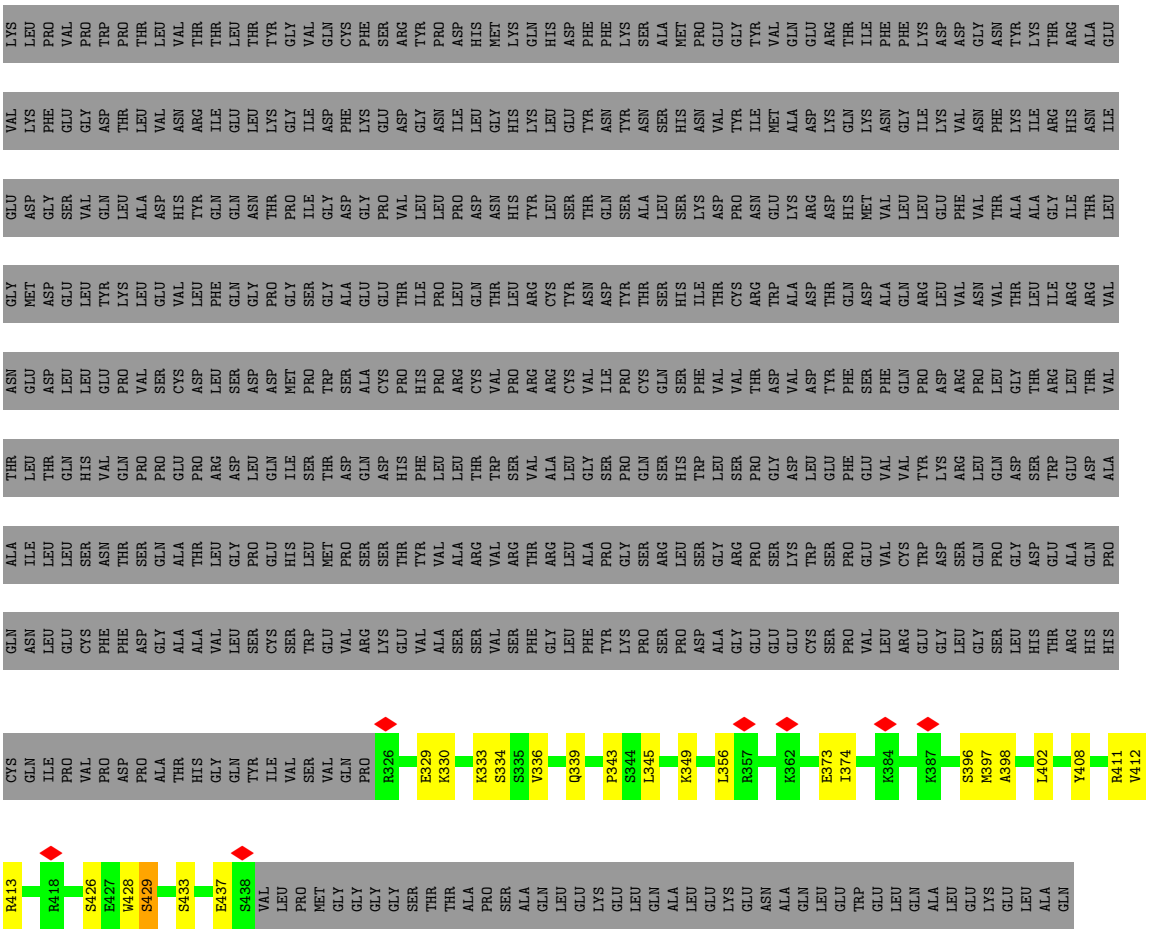
• Molecule 1: Cytokine receptor common subunit beta

Chain B:



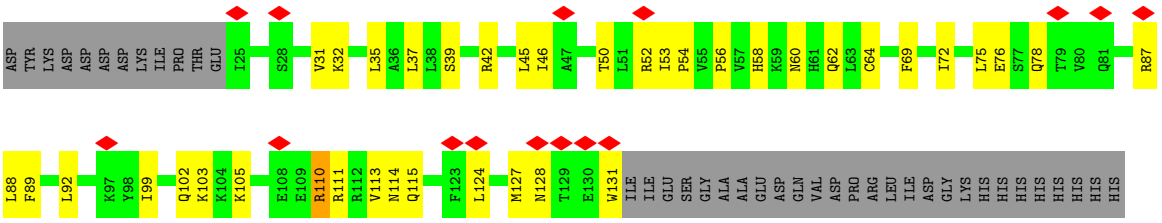
• Molecule 1: Cytokine receptor common subunit beta

Chain E:



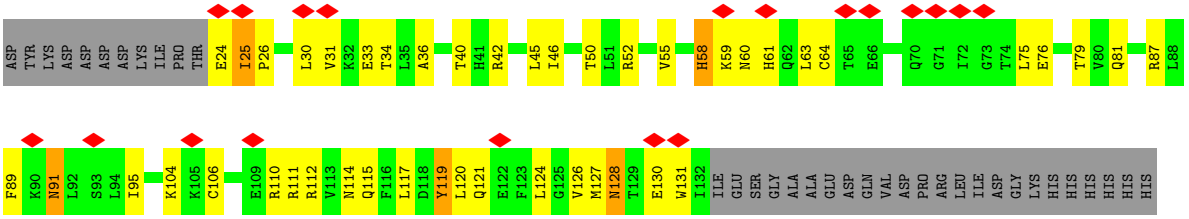
• Molecule 2: Interleukin-5

Chain C:



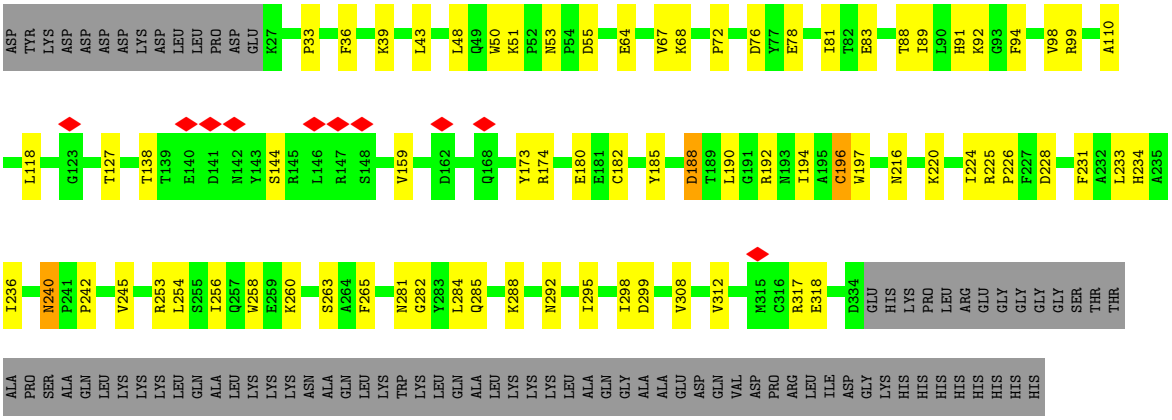
• Molecule 2: Interleukin-5

Chain D:



• Molecule 3: Interleukin-5 receptor subunit alpha

Chain F:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	418819	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 ($e^-/Å^2$)	59.9	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.277	Depositor
Minimum map value	-0.023	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.026	Depositor
Recommended contour level	0.126	Depositor
Map size (Å)	229.856, 229.856, 229.856	wwPDB
Map dimensions	176, 176, 176	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.306, 1.306, 1.306	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.28	0/777	0.54	0/1063
1	E	0.25	0/967	0.52	0/1309
2	C	0.38	1/875 (0.1%)	0.72	2/1180 (0.2%)
2	D	0.27	0/892	0.54	0/1203
3	F	0.27	0/2535	0.53	0/3458
All	All	0.29	1/6046 (0.0%)	0.56	2/8213 (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
2	C	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	54	PRO	CG-CD	-6.24	1.30	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	54	PRO	CA-N-CD	-12.51	93.99	111.50
2	C	54	PRO	N-CD-CG	-8.49	90.46	103.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	C	110	ARG	Sidechain

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	B	758	0	720	11	0
1	E	942	0	902	15	0
2	C	862	0	888	43	0
2	D	879	0	906	43	0
3	F	2471	0	2398	51	0
4	C	14	0	13	1	0
4	F	56	0	52	4	0
All	All	5982	0	5879	133	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 11.

The worst 5 of 133 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)
2:C:111:ARG:HD3	2:C:115:GLN:HB2	1.63	0.80
2:D:25:ILE:HD12	2:D:26:PRO:HD2	1.65	0.79
2:C:110:ARG:NH2	2:D:52:ARG:HD2	1.98	0.78
3:F:188:ASP:HB3	3:F:194:ILE:HD11	1.67	0.77
1:B:104:ASP:OD2	2:C:87:ARG:NH1	2.19	0.75

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	B	90/717 (13%)	86 (96%)	3 (3%)	1 (1%)	12 45
1	E	111/717 (16%)	109 (98%)	2 (2%)	0	100 100
2	C	105/146 (72%)	99 (94%)	5 (5%)	1 (1%)	13 46
2	D	107/146 (73%)	101 (94%)	5 (5%)	1 (1%)	14 48
3	F	306/392 (78%)	294 (96%)	12 (4%)	0	100 100
All	All	719/2118 (34%)	689 (96%)	27 (4%)	3 (0%)	32 63

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	78	MET
2	C	113	VAL
2	D	25	ILE

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	89/634 (14%)	87 (98%)	2 (2%)	47 69
1	E	102/634 (16%)	98 (96%)	4 (4%)	27 57
2	C	97/132 (74%)	96 (99%)	1 (1%)	73 85
2	D	99/132 (75%)	93 (94%)	6 (6%)	15 44
3	F	276/346 (80%)	268 (97%)	8 (3%)	37 63
All	All	663/1878 (35%)	642 (97%)	21 (3%)	36 61

5 of 21 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	144	SER
3	F	220	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	F	299	ASP
3	F	240	ASN
3	F	196	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	C	78	GLN
2	D	81	GLN

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)

5 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	$\#\|Z\| > 2$
4	NAG	F	504	3	14,14,15	0.26	0	17,19,21	0.55	0
4	NAG	C	200	2	14,14,15	0.69	1 (7%)	17,19,21	0.52	0
4	NAG	F	503	3	14,14,15	0.53	0	17,19,21	0.69	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	F	502	3	14,14,15	0.39	0	17,19,21	0.62	0
4	NAG	F	501	3	14,14,15	0.31	0	17,19,21	0.56	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	F	504	3	-	2/6/23/26	0/1/1/1
4	NAG	C	200	2	-	2/6/23/26	0/1/1/1
4	NAG	F	503	3	-	4/6/23/26	0/1/1/1
4	NAG	F	502	3	-	2/6/23/26	0/1/1/1
4	NAG	F	501	3	-	4/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	200	NAG	C1-C2	2.37	1.55	1.52

There are no bond angle outliers.

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	F	502	NAG	C4-C5-C6-O6
4	F	503	NAG	O5-C5-C6-O6
4	F	502	NAG	O5-C5-C6-O6
4	C	200	NAG	C4-C5-C6-O6
4	F	501	NAG	O5-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	200	NAG	1	0
4	F	503	NAG	1	0
4	F	501	NAG	3	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

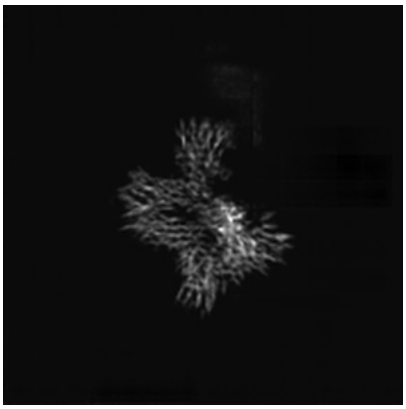
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41367. These allow visual inspection of the internal detail of the map and identification of artifacts.

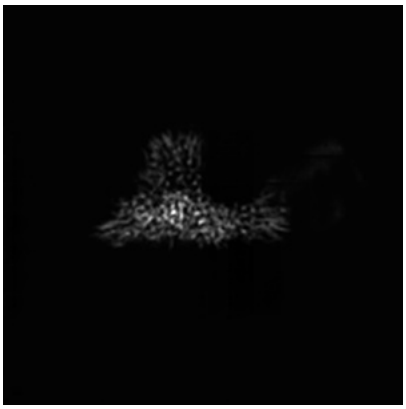
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

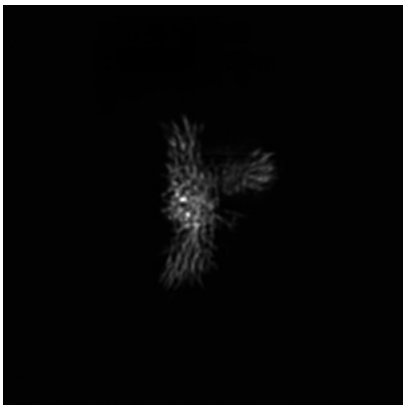
6.1.1 Primary map



X

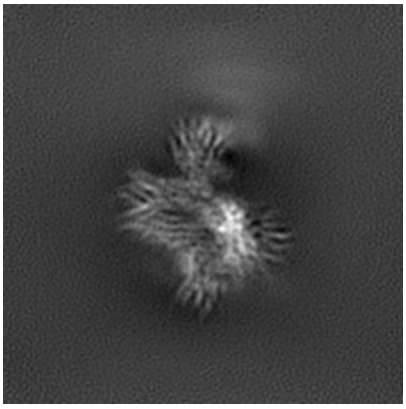


Y

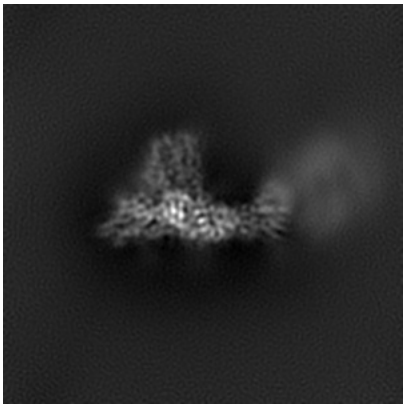


Z

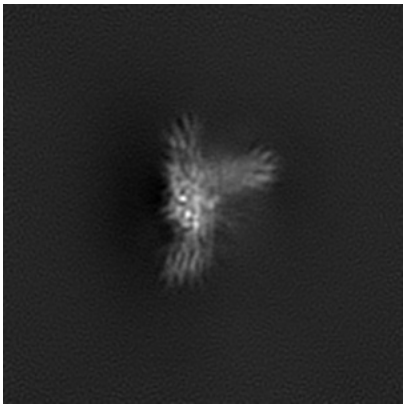
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

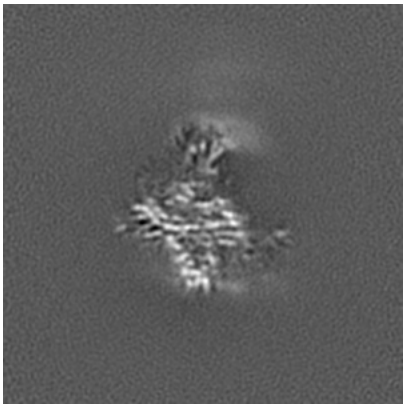
6.2.1 Primary map

X Index: 88

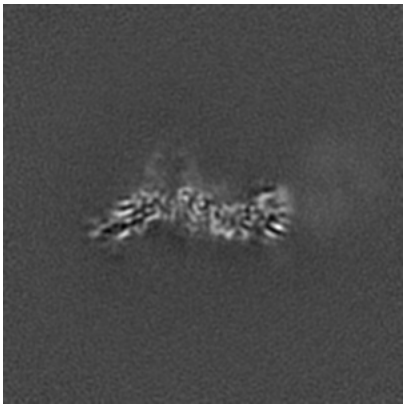
Y Index: 88

Z Index: 88

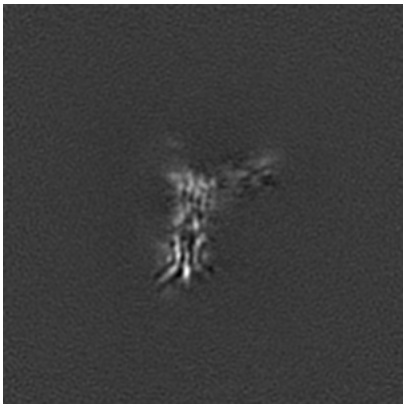
6.2.2 Raw map



X Index: 88



Y Index: 88



Z Index: 88

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

6.3 Largest variance slices (i)

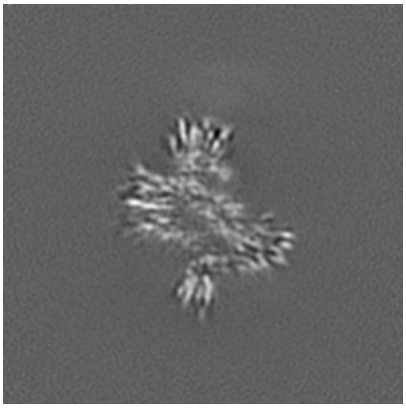
6.3.1 Primary map

X Index: 80

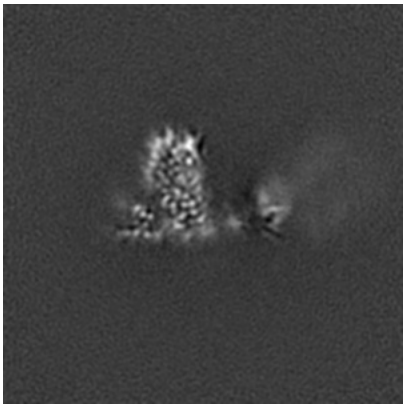
Y Index: 90

Z Index: 78

6.3.2 Raw map



X Index: 80



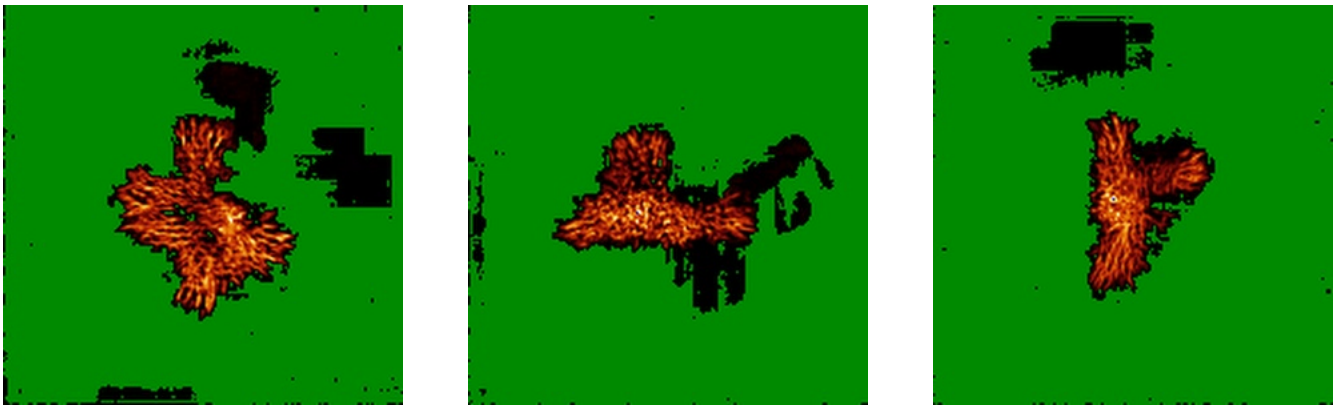
Y Index: 99

Z Index: 78

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

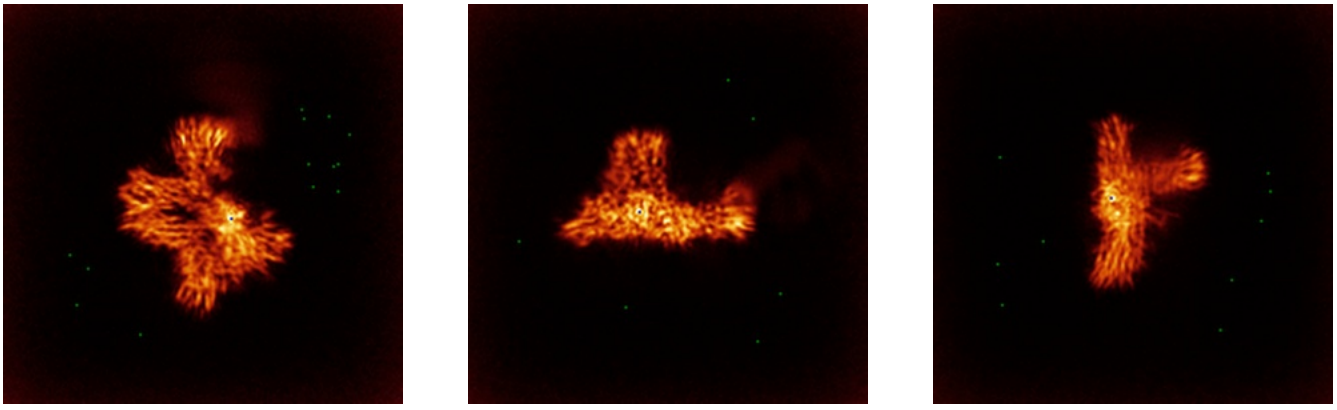
6.4 Orthogonal standard-deviation projections (False-color) (i)

6.4.1 Primary map



X Y Z

6.4.2 Raw map

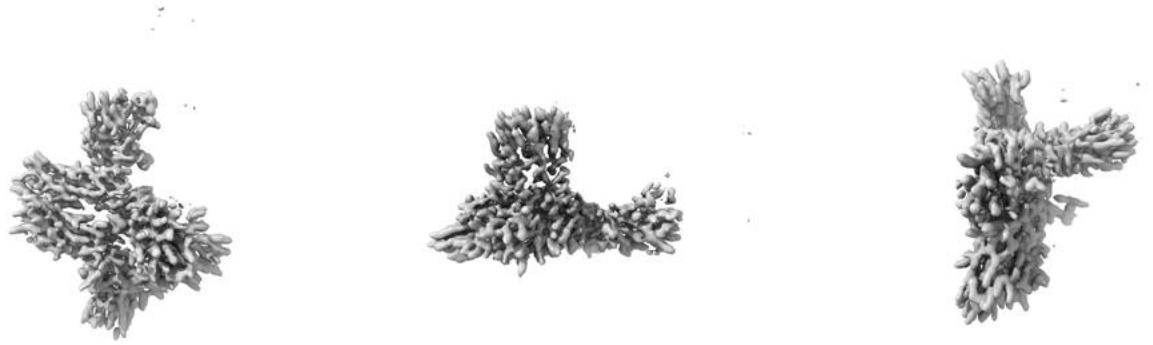


X Y Z

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

6.5 Orthogonal surface views (i)

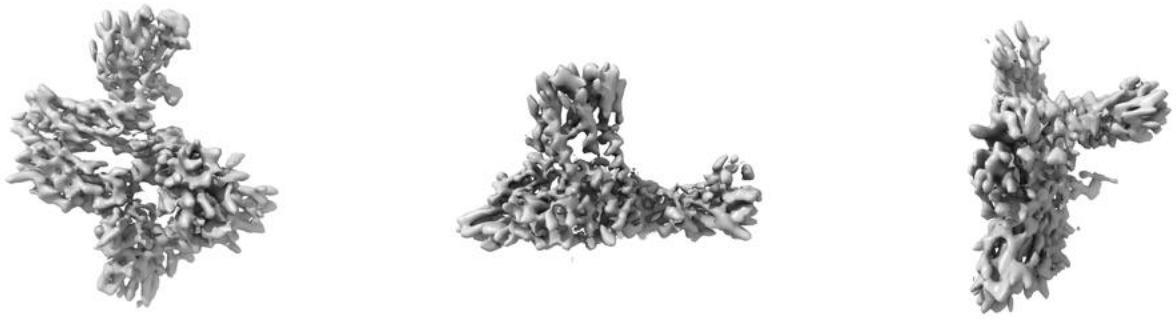
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.126. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

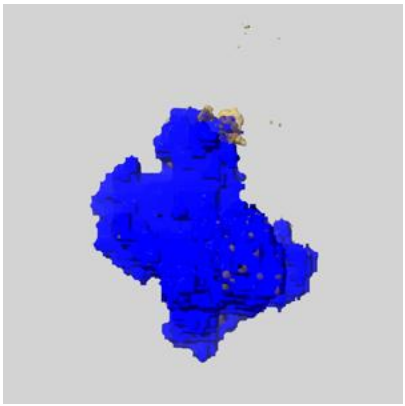
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

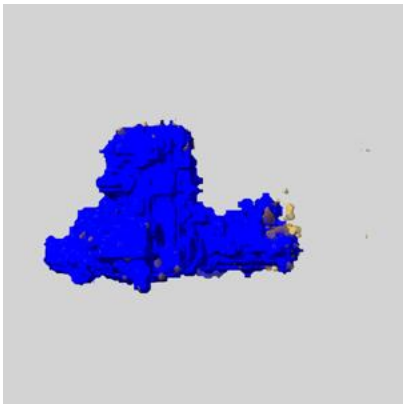
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

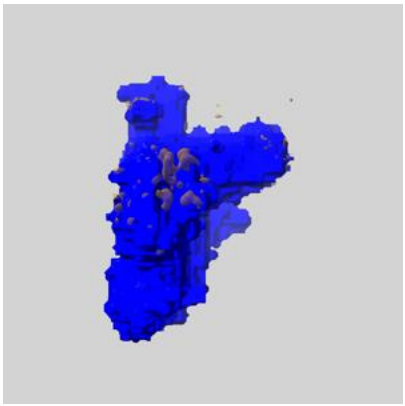
6.6.1 emd_41367_msk_1.map (i)



X



Y

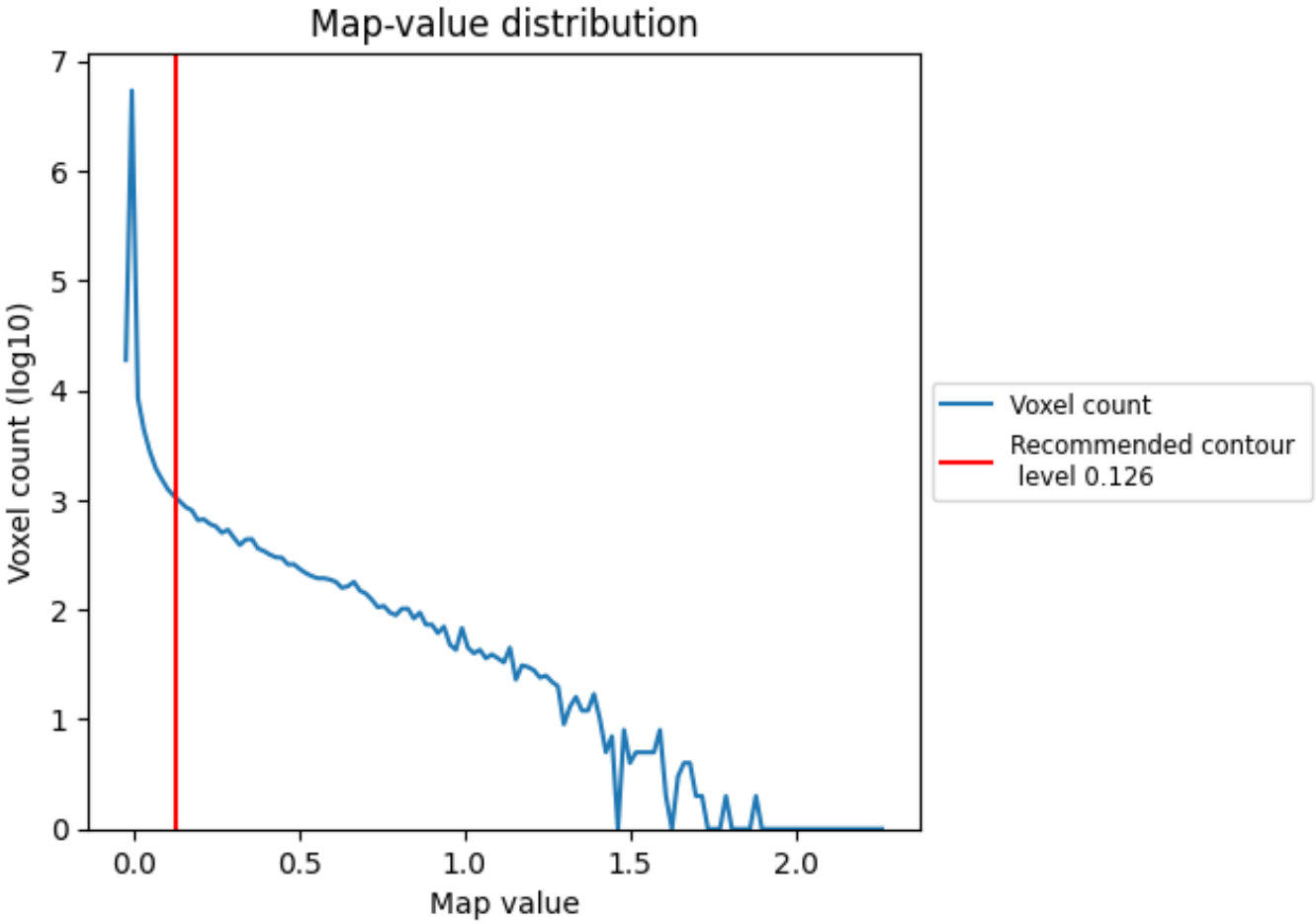


Z

7 Map analysis

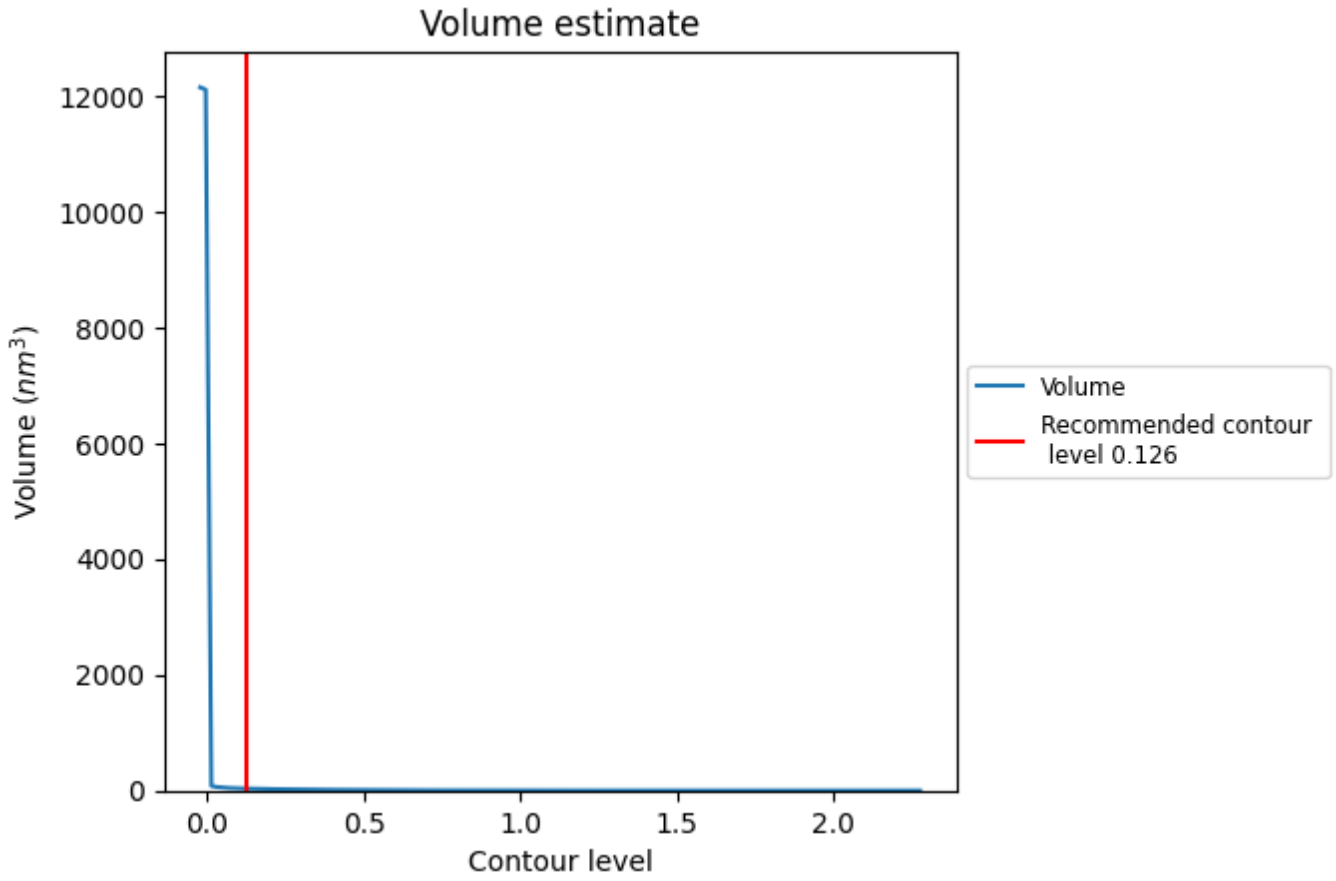
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

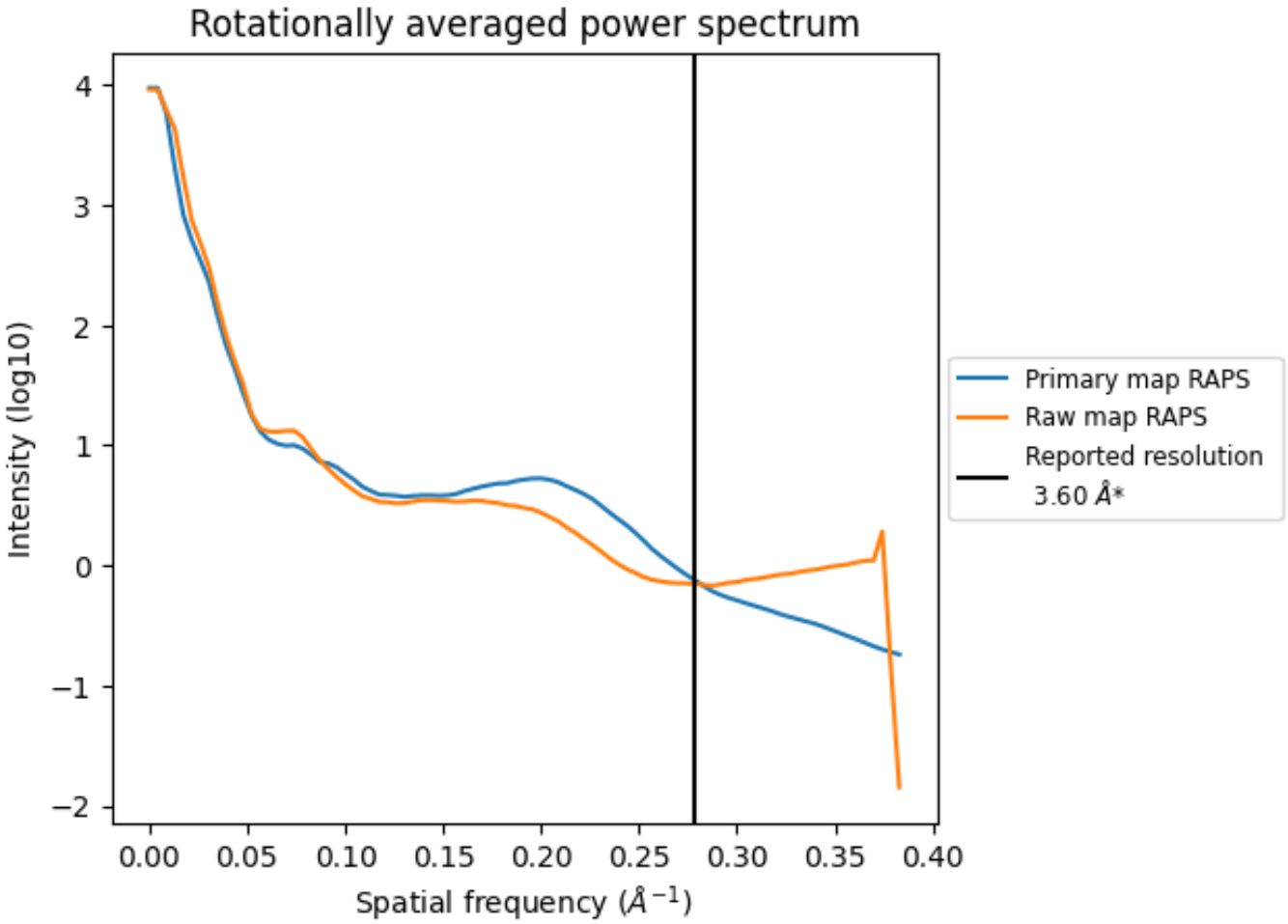
7.2 Volume estimate (i)



The volume at the recommended contour level is 34 nm^3; this corresponds to an approximate mass of 30 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)

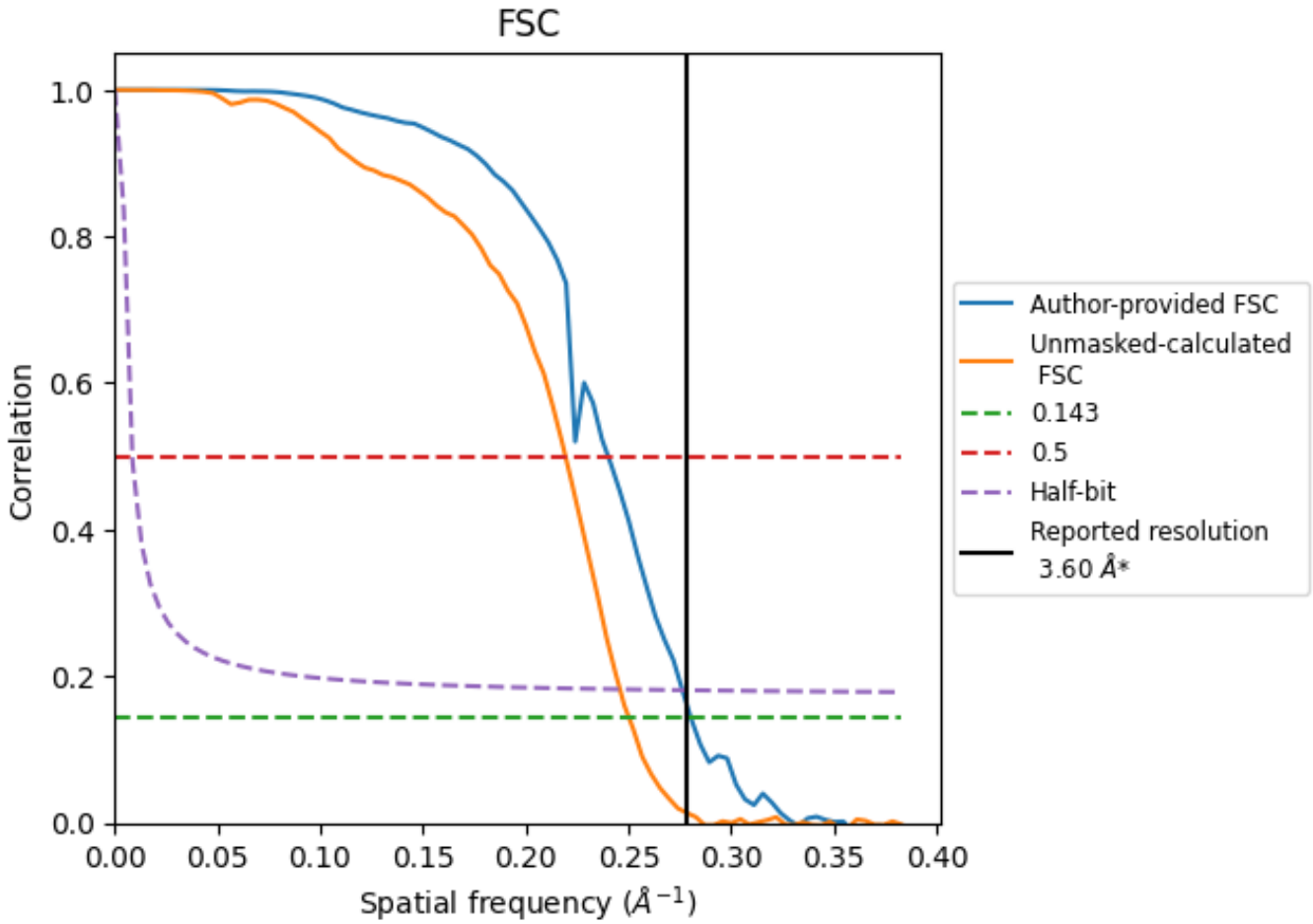


*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.278 Å^{-1}

8.2 Resolution estimates (i)

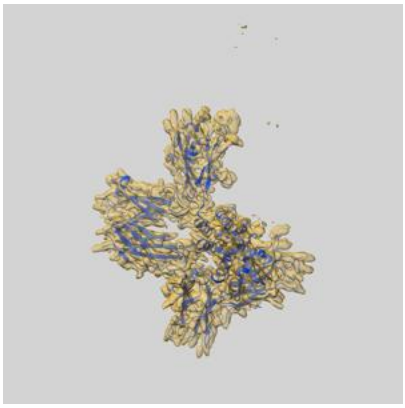
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.57	4.16	3.62
Unmasked-calculated*	4.00	4.56	4.07

*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 4.00 differs from the reported value 3.6 by more than 10 %

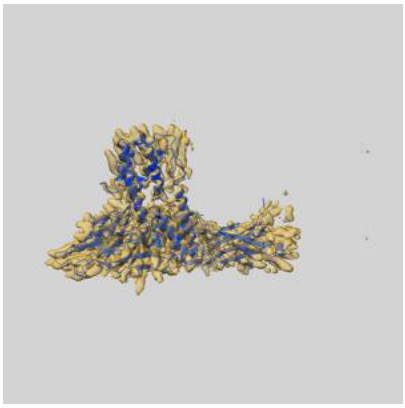
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41367 and PDB model 8TLD. Per-residue inclusion information can be found in section 3 on page 22.

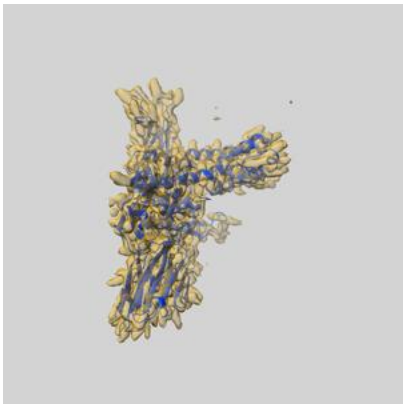
9.1 Map-model overlay



X



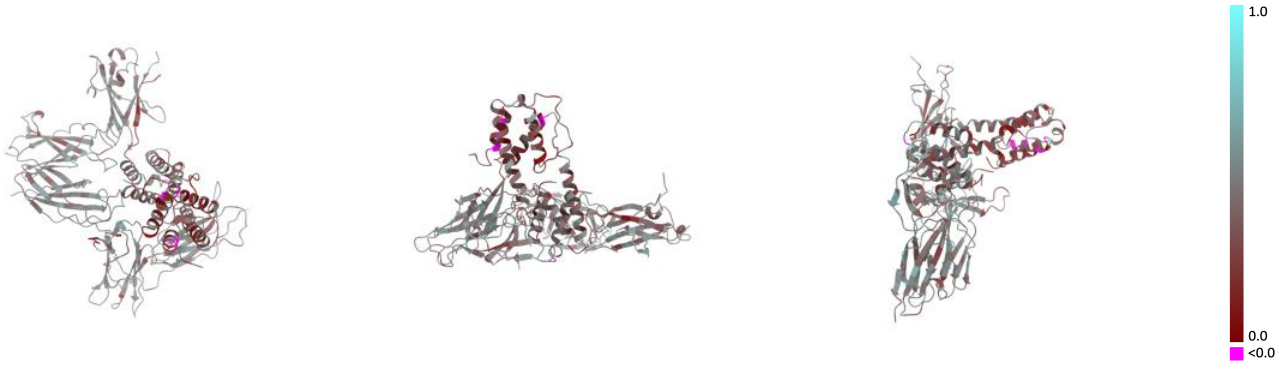
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.126 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.

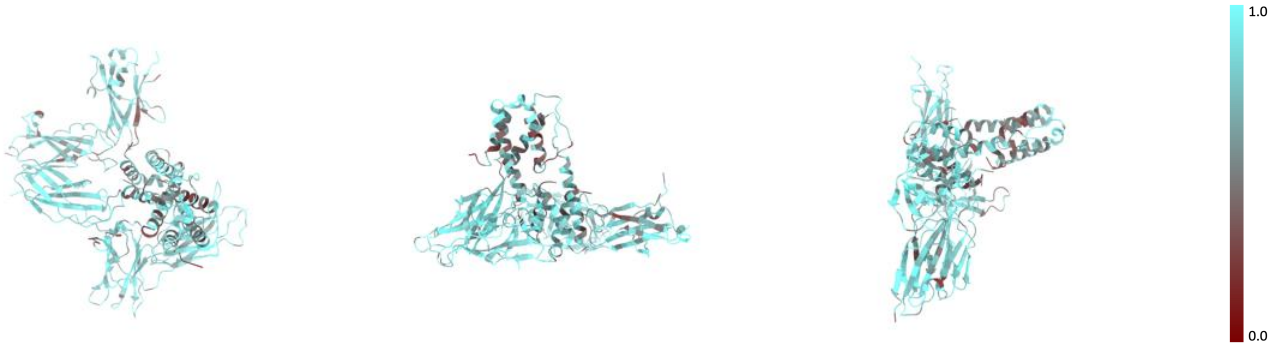
9.2 Q-score mapped to coordinate model (i)



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.

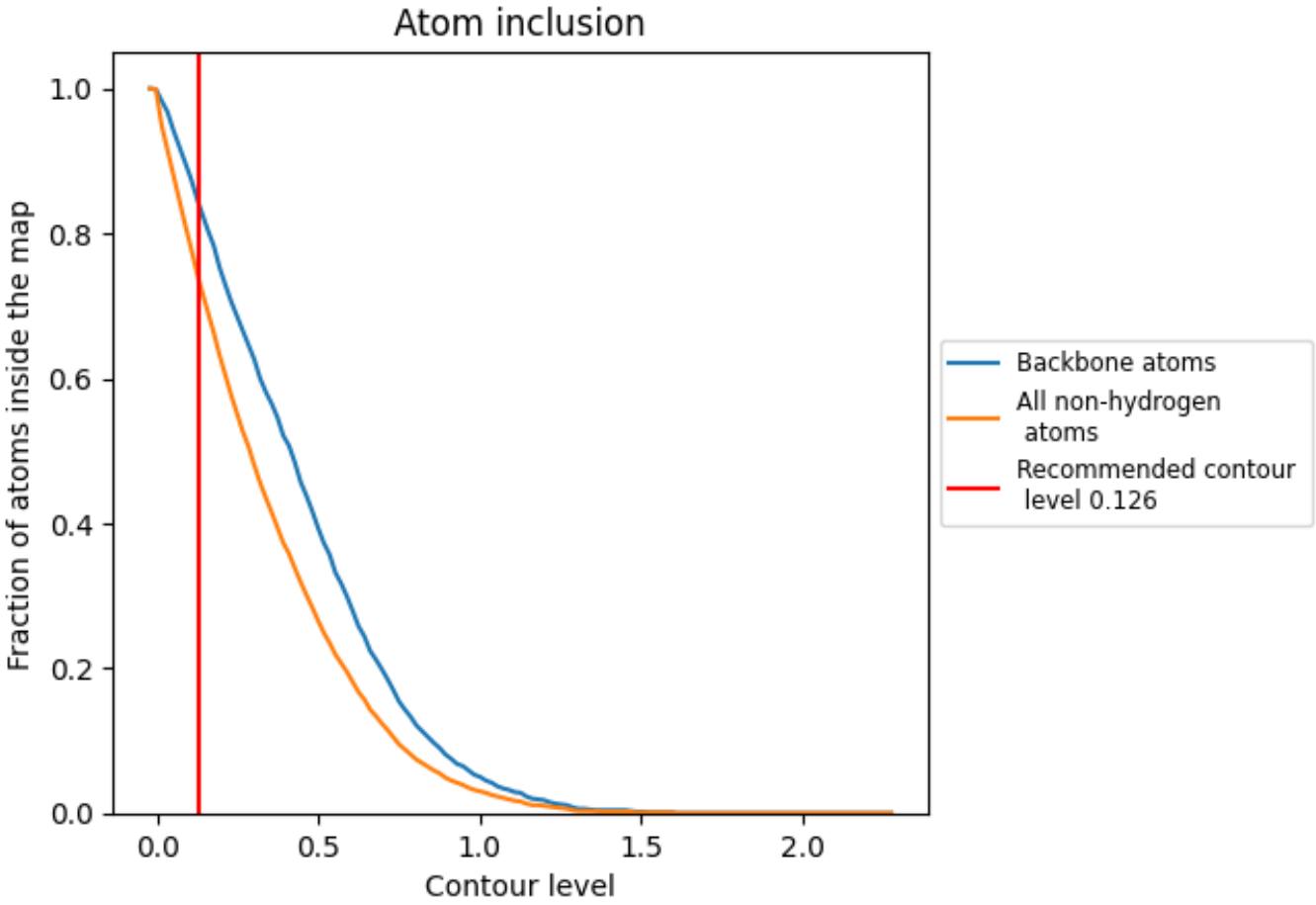
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.126).

9.4 Atom inclusion (i)



At the recommended contour level, 84% of all backbone atoms, 74% 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 (0.126) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7390	0.4090
B	0.7510	0.4330
C	0.6600	0.3500
D	0.6530	0.3100
E	0.7560	0.4460
F	0.7870	0.4420