



Full wwPDB EM Validation Report ⓘ

Mar 14, 2026 – 03:49 AM UTC

PDB ID : 8IVQ / pdb_00008ivq
EMDB ID : EMD-35759
Title : Cryo-EM structure of mouse BIRC6, Global map
Authors : Liu, S.; Jiang, T.; Bu, F.; Zhao, J.; Wang, G.; Li, N.; Gao, N.; Qiu, X.
Deposited on : 2023-03-28
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

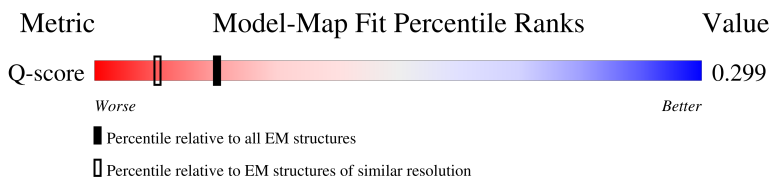
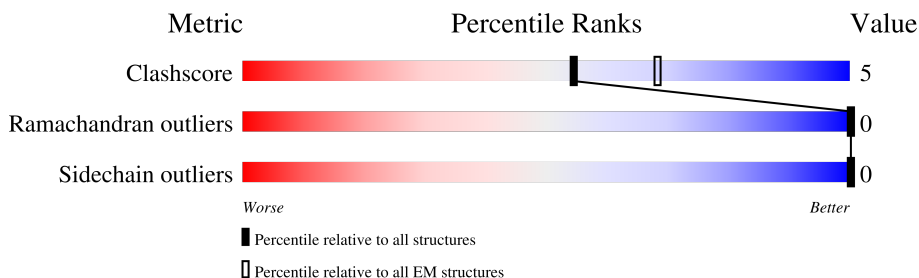
1 Overall quality at a glance

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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12797 (3.10 - 4.10)

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	4896	
1	B	4896	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 41900 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 Isoform 2 of Baculoviral IAP repeat-containing protein 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	2921	Total 20950	C 13236	N 3680	O 3904	S 130	0	0
1	B	2921	Total 20950	C 13236	N 3680	O 3904	S 130	0	0

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-50	MET	-	initiating methionine	UNP O88738
A	-49	ASP	-	expression tag	UNP O88738
A	-48	TYR	-	expression tag	UNP O88738
A	-47	LYS	-	expression tag	UNP O88738
A	-46	ASP	-	expression tag	UNP O88738
A	-45	HIS	-	expression tag	UNP O88738
A	-44	ASP	-	expression tag	UNP O88738
A	-43	GLY	-	expression tag	UNP O88738
A	-42	ASP	-	expression tag	UNP O88738
A	-41	TYR	-	expression tag	UNP O88738
A	-40	LYS	-	expression tag	UNP O88738
A	-39	ASP	-	expression tag	UNP O88738
A	-38	HIS	-	expression tag	UNP O88738
A	-37	ASP	-	expression tag	UNP O88738
A	-36	ILE	-	expression tag	UNP O88738
A	-35	ASP	-	expression tag	UNP O88738
A	-34	TYR	-	expression tag	UNP O88738
A	-33	LYS	-	expression tag	UNP O88738
A	-32	ASP	-	expression tag	UNP O88738
A	-31	ASP	-	expression tag	UNP O88738
A	-30	ASP	-	expression tag	UNP O88738
A	-29	ASP	-	expression tag	UNP O88738
A	-28	LYS	-	expression tag	UNP O88738
A	-27	ARG	-	expression tag	UNP O88738
A	-26	VAL	-	expression tag	UNP O88738
A	-25	VAL	-	expression tag	UNP O88738

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	PRO	-	expression tag	UNP O88738
A	-23	LEU	-	expression tag	UNP O88738
A	-22	GLU	-	expression tag	UNP O88738
A	-21	SER	-	expression tag	UNP O88738
A	-20	THR	-	expression tag	UNP O88738
A	-19	GLY	-	expression tag	UNP O88738
A	-18	LEU	-	expression tag	UNP O88738
A	-17	GLN	-	expression tag	UNP O88738
A	-16	GLU	-	expression tag	UNP O88738
A	-15	LEU	-	expression tag	UNP O88738
A	-14	ALA	-	expression tag	UNP O88738
A	-13	THR	-	expression tag	UNP O88738
A	-12	MET	-	expression tag	UNP O88738
A	-11	GLU	-	expression tag	UNP O88738
A	-10	GLN	-	expression tag	UNP O88738
A	-9	LYS	-	expression tag	UNP O88738
A	-8	LEU	-	expression tag	UNP O88738
A	-7	ILE	-	expression tag	UNP O88738
A	-6	SER	-	expression tag	UNP O88738
A	-5	GLU	-	expression tag	UNP O88738
A	-4	GLU	-	expression tag	UNP O88738
A	-3	ASP	-	expression tag	UNP O88738
A	-2	LEU	-	expression tag	UNP O88738
A	-1	GLU	-	expression tag	UNP O88738
A	0	PHE	-	expression tag	UNP O88738
A	178	ILE	THR	conflict	UNP O88738
A	690	THR	ALA	conflict	UNP O88738
A	2079	ARG	GLY	conflict	UNP O88738
A	2418	GLY	CYS	conflict	UNP O88738
A	2959	ILE	THR	conflict	UNP O88738
A	3226	THR	SER	conflict	UNP O88738
A	3914	VAL	MET	conflict	UNP O88738
A	3929	VAL	ILE	conflict	UNP O88738
A	4346	MET	VAL	conflict	UNP O88738
B	-50	MET	-	initiating methionine	UNP O88738
B	-49	ASP	-	expression tag	UNP O88738
B	-48	TYR	-	expression tag	UNP O88738
B	-47	LYS	-	expression tag	UNP O88738
B	-46	ASP	-	expression tag	UNP O88738
B	-45	HIS	-	expression tag	UNP O88738
B	-44	ASP	-	expression tag	UNP O88738
B	-43	GLY	-	expression tag	UNP O88738

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	-42	ASP	-	expression tag	UNP O88738
B	-41	TYR	-	expression tag	UNP O88738
B	-40	LYS	-	expression tag	UNP O88738
B	-39	ASP	-	expression tag	UNP O88738
B	-38	HIS	-	expression tag	UNP O88738
B	-37	ASP	-	expression tag	UNP O88738
B	-36	ILE	-	expression tag	UNP O88738
B	-35	ASP	-	expression tag	UNP O88738
B	-34	TYR	-	expression tag	UNP O88738
B	-33	LYS	-	expression tag	UNP O88738
B	-32	ASP	-	expression tag	UNP O88738
B	-31	ASP	-	expression tag	UNP O88738
B	-30	ASP	-	expression tag	UNP O88738
B	-29	ASP	-	expression tag	UNP O88738
B	-28	LYS	-	expression tag	UNP O88738
B	-27	ARG	-	expression tag	UNP O88738
B	-26	VAL	-	expression tag	UNP O88738
B	-25	VAL	-	expression tag	UNP O88738
B	-24	PRO	-	expression tag	UNP O88738
B	-23	LEU	-	expression tag	UNP O88738
B	-22	GLU	-	expression tag	UNP O88738
B	-21	SER	-	expression tag	UNP O88738
B	-20	THR	-	expression tag	UNP O88738
B	-19	GLY	-	expression tag	UNP O88738
B	-18	LEU	-	expression tag	UNP O88738
B	-17	GLN	-	expression tag	UNP O88738
B	-16	GLU	-	expression tag	UNP O88738
B	-15	LEU	-	expression tag	UNP O88738
B	-14	ALA	-	expression tag	UNP O88738
B	-13	THR	-	expression tag	UNP O88738
B	-12	MET	-	expression tag	UNP O88738
B	-11	GLU	-	expression tag	UNP O88738
B	-10	GLN	-	expression tag	UNP O88738
B	-9	LYS	-	expression tag	UNP O88738
B	-8	LEU	-	expression tag	UNP O88738
B	-7	ILE	-	expression tag	UNP O88738
B	-6	SER	-	expression tag	UNP O88738
B	-5	GLU	-	expression tag	UNP O88738
B	-4	GLU	-	expression tag	UNP O88738
B	-3	ASP	-	expression tag	UNP O88738
B	-2	LEU	-	expression tag	UNP O88738
B	-1	GLU	-	expression tag	UNP O88738

Continued on next page...

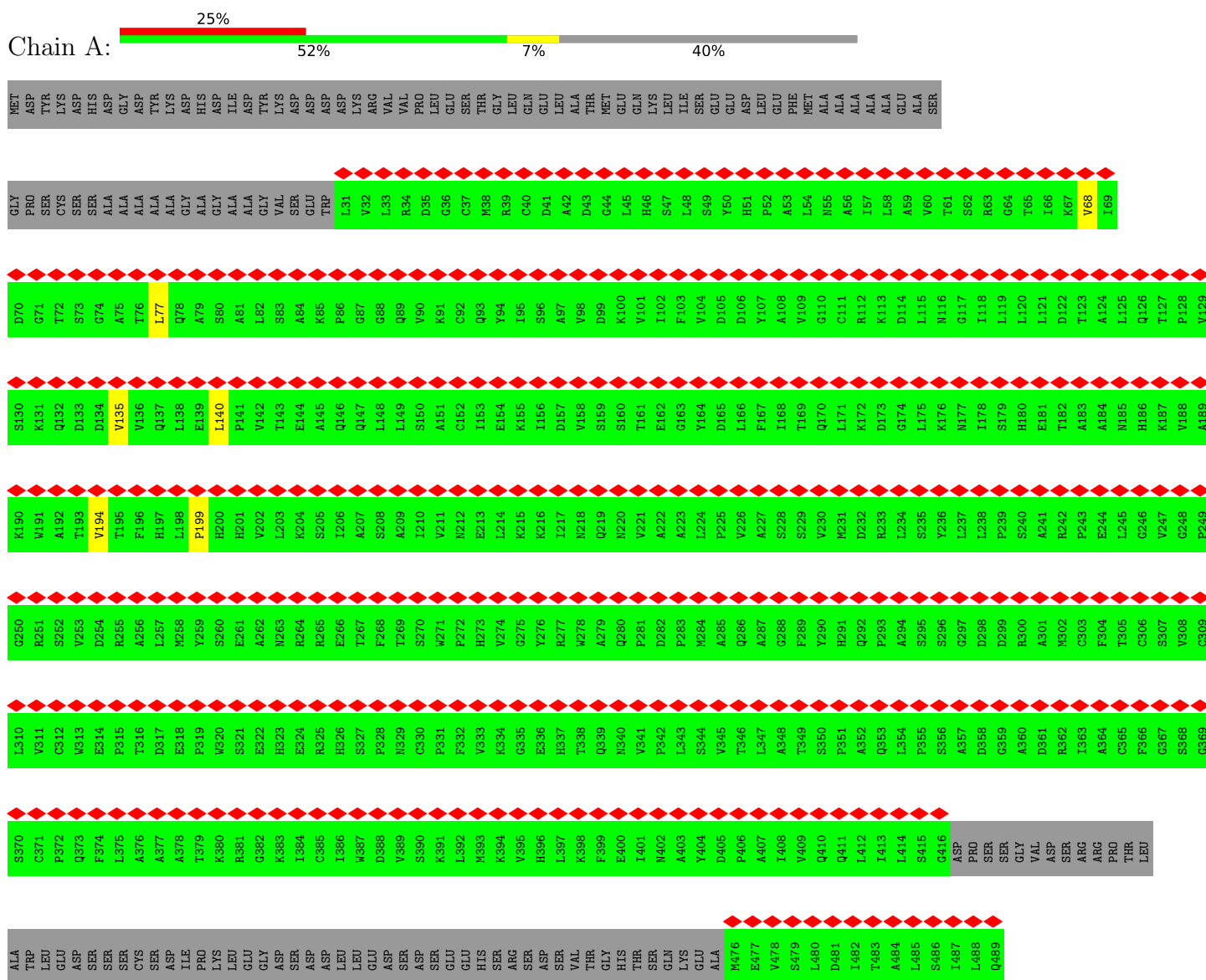
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	PHE	-	expression tag	UNP O88738
B	178	ILE	THR	conflict	UNP O88738
B	690	THR	ALA	conflict	UNP O88738
B	2079	ARG	GLY	conflict	UNP O88738
B	2418	GLY	CYS	conflict	UNP O88738
B	2959	ILE	THR	conflict	UNP O88738
B	3226	THR	SER	conflict	UNP O88738
B	3914	VAL	MET	conflict	UNP O88738
B	3929	VAL	ILE	conflict	UNP O88738
B	4346	MET	VAL	conflict	UNP O88738

3 Residue-property plots

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: Isoform 2 of Baculoviral IAP repeat-containing protein 6







VAL	GLN	L3846	SER	GLU	G3551	T3209	LEU	L2915	L2798	A2552
ILE	SER	P3847	HIS	ILE	I3552	H3210	ASP	R2929	N2656	L2553
THR	SER	V3848	SER	ALA	I3553	L3218	A3015	P2930	S2657	D2554
ASP	ARG	S3849	ALA	GLN	PRO	L3218	Y3061	SER	SER	A2555
PRO	ALA	T3850	ALA	SER	PRO	P3222	M3052	VAL	GLY	R2556
LEU	VAL	S3853	THR	VAL	PRO	E3228	Q3055	THR	ASN	L2557
SER	ASP	D3854	THR	ASP	VAL	N3389	G3056	THR	THR	E2558
THR	SER	V3736	THR	GLN	VAL	N3395	T3060	THR	ASN	
LYS	GLN	R3858	GLN	SER	CYS	D3396	T3060	THR	THR	E2562
THR	ASP	V3859	ASP	GLN	HIS	P3397	V3112	THR	ASN	Q2563
ASP	ARG	S3860	THR	ASP	HIS	L3239	S3113	THR	GLY	Q2564
PRO	LYS	D3861	LYS	LEU	LEU	T3398	T3114	ASP	ALA	A2565
ARG	PRO	T3862	ARG	SER	SER	T3241	F3118	VAL	ASP	T2566
LYS	ARG	P3863	ARG	MET	MET	L3255	L3119	SER	ASP	L2567
LEU	THR	SER	ARG	THR	THR	L3400	D3120	GLU	GLY	
HIS	ARG	SER	HIS	HIS	ASP	N3401	L3118	GLU	A2674	P2578
PRO	ILE	THR	ILE	VAL	ASP	L3405	L3119	GLU	N2675	
GLU	ARG	THR	THR	PRO	ASP	L3405	D3120	GLU	V2853	
LYS	GLN	ALA	ALA	GLN	SER	R3408	SER	VAL	D2861	L2584
ASP	LYS	LYS	LYS	LYS	LYS	L3409	GLY	VAL	K2862	
LEU	LEU	LEU	THR	GLN	GLN	N3410	THR	GLY	L2701	T2585
SER	GLY	SER	THR	ASP	ASP	G3411	PRO	GLY	L2702	R2586
GLN	ILE	GLU	T3777	LEU	LEU	L3412	ASN	LYS	R2866	
VAL	GLY	ALA	ALA	SER	SER	S3280	ALA	ASP	C2706	T2587
GLY	SER	PRO	PRO	SER	SER	K3283	VAL	VAL	GLY	S2588
LYS	GLN	LYS	GLN	LEU	SER	L3284	VAL	ASN	SER	PRO
ASP	ASP	ASP	ARG	SER	SER	L3285	ASP	GLY	ASP	THR
LYS	LYS	GLY	GLY	THR	THR	L3418	THR	SER	SER	PHE
GLU	SER	LEU	LEU	ASP	ASP	K3433	LYS	ALA	ALA	GLN
LYS	ALA	THR	THR	LYS	LYS	G3456	THR	THR	GLY	PRO
ASN	HIS	SER	SER	ASN	ALA	R3457	ARG	PRO	ILE	GLY
GLU	GLU	GLU	GLU	GLN	ALA	M457	ILE	GLY	GLY	THR
LYS	LYS	LYS	LYS	ALA	GLN	G3456	ILE	GLY	GLY	LEU
GLY	ILE	ILE	ILE	ALA	ALA	R3457	ARG	GLY	GLY	LEU
THR	THR	THR	SER	LEU	LEU	T3293	THR	SER	PHE	LEU
ASN	ASN	ASN	ASN	ASN	ASN	A3295	LYS	ALA	ALA	GLY
GLU	GLU	GLU	GLU	GLN	ALA	THR	THR	ALA	ASN	ASN
LYS	LYS	LYS	LYS	ALA	ALA	VAL	THR	GLU	LEU	ASN
GLY	ILE	ILE	ILE	ALA	ALA	THR	THR	GLU	LEU	ASN
ILE	ILE	ILE	ILE	ALA	ALA	VAL	THR	GLU	LEU	ASN
ASP	ASP	ASP	ASP	LEU	LEU	G3456	THR	GLU	LEU	ASN
GLU	GLU	GLU	GLU	LEU	LEU	R3457	THR	GLU	LEU	ASN
GLY	GLY	GLY	GLY	LEU	LEU	M457	THR	GLU	LEU	ASN
THR	THR	THR	THR	LEU	LEU	T3293	THR	GLU	LEU	ASN
GLU	GLU	GLU	GLU	LEU	LEU	L3293	THR	GLU	LEU	ASN
GLY	GLY									



GLY	PRO	SER	CYS	SER	SER	ALA	ALA	ALA	ALA	ALA	GLY	GLY	GLY	GLY	VAL	SER	GLU	TRP	L31	V32	L33	R34	D35	G36	C37	N38	R39	C40	D41	A42	D43	G44	L45	H46	S47	L48	S49	Y50	H51	P52	A53	L54	N55	A56	I57	L58	A59	V60	T61	S62	R63	G64	T65	I66	K67	K68	I69			
D70	G71	T72	S73	G74	A75	T76	L77	Q78	L78	A79	S80	A81	L82	S83	A84	K85	P86	G87	G88	Q89	V90	K91	C92	Q93	Y94	I95	S96	A97	V98	D99	K100	V101	I102	F103	V104	D105	D106	Y107	A108	V109	G110	C111	R112	K113	L114	L115	N116	G117	L118	L119	T120	L121	D122	T123	A124	L125	Q126	T127	P128	V129
S130	K131	Q132	D133	L134	V135	V136	Q137	L138	E139	L140	P141	V142	T143	E144	A145	Q146	T147	L148	L149	S150	A151	C152	I153	E154	K155	I156	D157	V158	S159	S160	T161	E162	G163	Y164	D165	L166	F167	I168	T169	Q170	L171	K172	D173	G174	L175	K176	N177	L178	S179	H180	E181	T182	A183	A184	N185	H186	K187	V188	A189	
K190	W191	T192	T193	V194	T195	F196	H197	L198	P199	H200	H201	V202	L203	K204	S205	L206	T207	F208	A209	I210	V211	N212	E213	L214	K215	K216	T217	N218	Q219	N220	V221	A222	G223	L224	P225	V226	A227	S228	S229	V230	H231	D232	R233	L234	S235	Y236	L237	L238	P239	S240	A241	R242	E243	E244	L245	G246	G247	G248	P249	
G250	R251	S252	V253	D254	R255	A256	L257	M258	V259	S260	E261	A262	N263	A264	R265	E266	T267	F268	T269	S270	W271	P272	H273	V274	G275	Y276	R277	N278	A279	Q280	P281	D282	M283	A284	A285	Q286	G287	G288	F289	Y290	H291	Q292	P293	A294	S295	S296	G297	D298	D299	R300	A301	N302	C303	F304	T305	C306	S307	V308	C309	
L310	V311	C312	W313	E314	P315	A316	D317	E318	P319	W320	S321	A322	H323	E324	R325	H326	S327	P328	N329	C330	P331	F332	V333	K334	G335	E336	H337	T338	Q339	N340	V341	P342	L343	S344	V345	T346	L347	A348	T349	P350	P351	A352	Q353	L354	P355	S356	A357	D358	G359	A360	D361	R362	T363	A364	C365	F366	V367	S368	G369	
S370	C371	P372	Q373	F374	L375	A376	A377	A378	T379	K380	R381	G382	K383	I384	C385	L386	W387	D388	V389	S390	K391	L392	M393	K394	V395	H396	L397	K398	F399	E400	L401	N402	A403	Y404	D405	P406	A407	I408	V409	Q410	Q411	L412	L413	L414	S415	G416	ASP	PRO	SER	GLY	VAL	ASP	SER	ARG	PRO	THR	LEU			
ALA	TRP	LEU	GLU	ASP	SER	SER	ALA	ALA	ALA	PRO	LYS	LEU	GLN	GLY	ASP	ASP	LEU	GLU	GLU	ASP	ASN	GLU	ILE	HIS	ARG	SER	ASP	VAL	THR	GLY	HIS	THR	ASN	GLN	LYS	GLU	ALA	M476	E477	V478	S479	L480	D481	I482	T483	A484	L485	S486	I487	L488	Q489									
Q490	P491	E492	LYS	LEU	TRP	GLN	TRP	GLU	ILE	VAL	ASN	VAL	LEU	GLU	ASP	LEU	GLU	GLU	GLY	ALA	ASN	PRO	ILE	GLU	ASN	SER	GLU	LYS	THR	LYS	THR	GLY	ASN	GLN	GLU	GLN	H535	N536	I537	F538	F539	P540	C541	L542	L543	A544	G545	G546	L547	L548	T549									
Y550	K551	S552	PRO	ALA	THR	GLN	LYS	PRO	ALA	GLY	ASN	SER	HIS	ARG	ASP	LEU	ARG	THR	GLY	GLU	SER	ILE	THR	GLN	GLY	THR	ASN	GLU	LYS	THR	ASN	THR	GLN	GLU	ASN	SER	PRO	VAL	R599	R600	T601	L602	P603	V604	L605	L606	L607	Y608	S609											
I610	K611	E612	S613	ASP	GLU	LYS	ALA	GLY	LYS	PHE	SER	ASN	S683	V684	P685	P686	K687	P688	G689	T690	L691	V692	Q693	C694	L695	R696	L697	P698	K699	F700	A701	E702	E703	E704	T705	L706	C707	I708	D709	S710	I711	T712	P713	TYR	C714	A715	D716	G717	I718	H719	L720	L721	V722	G723	L724	R725	T726	C727	SER	VAL
GLU	SER	LEU	SER	ALA	ASN	ILE	ASN	GLN	VAL	ALA	ASN	ASN	LYS	ASN	LEU	ASN	SER	ALA	ASN	CYS	ASN	ARG	ARG	LYS	ASP	LEU	GLU	SER	VAL	VAL	ASN	GLY	ALA	LEU	ILE	VAL	GLN	HIS	GLU	SER	PRO	ALA	ASP	VAL	PRO	GLU	HIS	LEU	LEU	ILE	ARG									
PRO	GLU	GLN	ARG	ASN	VAL	V796	S797	G798	G799	Y800	L801	Y802	L803	Y804	K805	H806	H807	Y808	T809	T810	R811	I812	H813	T814	L815	E816	E817	E818	P819	Y820	K821	I822	Q823	H824	I825	K826	D827	P828	Q829	D830	T831	I832	T833	S834	L835	I836	L837	L838	P839	P840	D841	I842	L843	D844	N845	ARG	GLU	ASP		







S4361	S4362	Y4363	L4364	ARG	ASN	D4367	S4368	Y4369	L4370	D4371	H4372	A4373	R4374	H4375	V4376	P4377	L4378	Y4379	R4380	A4381	L4382	L4383	E4384	L4385	L4386	R4387	A4388	I4389	A4390	S4391	C4392	T4393	S4394	M4395	V4396	P4397	L4398	L4399	LEU	PRO	LEU	SER	THR	GLU	ASN	GLY	GLU	GLU	GLU	ASP	GLN	SER	GLN	CYS	THR	S4420			
V4421	G4422	T4423	L4424	L4425	A4426	K4427	M4428	K4429	T4430	C4431	V4432	D4433	T4434	Y4435	T4436	N4437	R4438	L4439	R4440	S4441	K4442	ARG	GLU	ASN	LYS	VAL	LYS	ALA	GLY	VAL	LYS	PRO	ASP	S4394	ASP	GLN	GLU	PRO	GLY	GLY	LEU	A4463	L4464	L4465	V4466	P4467	D4468	I4469	Q4470	R4471	T4472	A4473	E4474	I4475	V4476	H4477	A4478	A4479	T4480
A4481	M4482	L4483	R4484	Q4485	ALA	ASN	GLN	GLU	LYS	LYS	GLY	GLU	ASP	TYR	SER	LYS	VAL	MET	LYS	PRO	LYS	PRO	LEU	VAL	LEU	LYS	SER	GLU	GLU	THR	GLU	VAL	LYS	LYS	LEU	GLN	PHE	ASP	THR	PHE	GLU	MET	VAL	SER	GLU	ASP	ASP	GLY	LYS	LEU	GLY								
PHE	LYS	VAL	ASN	TYR	HIS	TYR	MET	SER	GLN	VAL	LYS	ASN	ASP	ALA	ASN	SER	LYS	VAL	ALA	VAL	MET	LYS	ARG	ALA	LEU	VAL	THR	SER	GLU	THR	SER	GLU	VAL	PRO	LEU	VAL	THR	CYS	ASP	THR	PHE	GLU	MET	VAL	SER	GLU	ASP	ASP	GLY	LYS	LEU	GLY							
ILE	THR	GLY	PRO	ALA	ASP	THR	PRO	TYR	ASN	ALA	GLY	GLN	PHE	VAL	TYR	VAL	ARG	PRO	ARG	LYS	PRO	GLM	GLU	ALA	VAL	THR	SER	GLU	THR	SER	GLU	PRO	GLY	GLY	THR	PRO	ASN	VAL	THR	CYS	ASP	GLU	GLU	VAL	ARG	LEU	ASP	ILE	MET	LYS	VAL	LEU	THR						
TRP	HIS	ARG	PRO	GLY	GLU	GLU	LYS	TRP	ASN	GLN	PRO	GLN	PHE	VAL	GLN	SER	VAL	ASN	PRO	LEU	ILE	PRO	GLU	ALA	VAL	VAL	THR	GLY	GLY	GLY	HIS	LEU	GLU	ARG	GLY	THR	PRO	ASN	VAL	THR	PRO	ASN	GLY	THR	GLN	SER	LYS	ARG	GLU	TYR	ASP	ILE	ASN	ILE	ARG				
GLN	ALA	THR	VAL	LYS	TRP	ALA	MET	LEU	GLN	ILE	ARG	ASN	PRO	PRO	SER	PHE	LEU	GLN	VAL	LEU	ILE	VAL	ALA	GLU	PRO	GLU	TYR	PHE	ASN	GLU	GLY	ALA	GLY	ASP	GLY	THR	PRO	GLN	THR	GLN	SER	LYS	ARG	GLU	TYR	ASP	ILE	ASN	ILE	ARG									
HIS	ALA	ALA	ALA	LEU	LYS	ARG	HIS	THR	ALA	GLN	LEU	ARG	GLU	GLU	LEU	LYS	LEU	PRO	CYS	PRO	GLU	GLY	LEU	ASP	PRO	ASP	ILE	GLU	ASP	ALA	ILE	SER	PRO	VAL	CYS	ARG	ALA	THR	GLY	ILE	THR	HIS	ASP	GLY	ASP	THR	LEU	ASP	LEU	PRO									
SER	ASP	PHE	GLN	LEU																																																							

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	154000	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 ($e^-/\text{\AA}^2$)	68.4	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.180	Depositor
Minimum map value	-0.086	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.03	Depositor
Map size ($\text{\AA}$)	438.4, 438.4, 438.4	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.37, 1.37, 1.37	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.24	0/21276	0.54	5/28980 (0.0%)
1	B	0.24	0/21276	0.54	4/28980 (0.0%)
All	All	0.24	0/42552	0.54	9/57960 (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	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	B	1396	PRO	CA-N-CD	-5.95	103.67	112.00
1	A	1396	PRO	CA-N-CD	-5.93	103.70	112.00
1	A	4321	MET	CA-CB-CG	5.34	124.79	114.10
1	B	4321	MET	CA-CB-CG	5.32	124.75	114.10
1	A	4305	GLU	CA-CB-CG	5.23	124.57	114.10
1	B	4305	GLU	CA-CB-CG	5.22	124.54	114.10
1	A	4162	LEU	CB-CG-CD2	-5.06	95.51	110.70
1	B	4162	LEU	CB-CG-CD2	-5.05	95.53	110.70
1	A	2638	VAL	N-CA-CB	-5.02	106.51	112.39

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1396	PRO	Peptide
1	A	1834	ILE	Peptide
1	B	1396	PRO	Peptide
1	B	1834	ILE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	20950	0	19684	215	0
1	B	20950	0	19684	224	0
All	All	41900	0	39368	413	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (413) 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:B:3798:PHE:O	1:B:3802:MET:HB3	1.81	0.81
1:A:3798:PHE:O	1:A:3802:MET:HB3	1.81	0.80
1:B:1383:ARG:HH21	1:B:2562:GLU:HB2	1.52	0.74
1:A:1383:ARG:HH21	1:A:2562:GLU:HB2	1.52	0.73
1:A:2375:GLY:HA2	1:A:2641:VAL:HA	1.76	0.68
1:A:1349:GLU:O	1:A:1353:CYS:HB2	1.94	0.67
1:B:2375:GLY:HA2	1:B:2641:VAL:HA	1.76	0.67
1:B:1349:GLU:O	1:B:1353:CYS:HB2	1.94	0.66
1:A:1417:PRO:HG2	1:A:2001:ILE:HG12	1.78	0.65
1:B:1417:PRO:HG2	1:B:2001:ILE:HG12	1.78	0.65
1:A:2703:ARG:NH1	1:A:2706:CYS:SG	2.71	0.64
1:B:1298:MET:HG2	1:B:1336:LEU:HD21	1.80	0.64
1:B:2703:ARG:NH1	1:B:2706:CYS:SG	2.71	0.63
1:B:3353:MET:SD	1:B:3408:ARG:NH2	2.72	0.63
1:A:3353:MET:SD	1:A:3408:ARG:NH2	2.72	0.63
1:A:1298:MET:HG2	1:A:1336:LEU:HD21	1.80	0.62
1:B:1169:ASP:HA	1:B:2567:LEU:HD21	1.83	0.61
1:B:1789:ASP:HB2	1:B:1865:TYR:HB2	1.82	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1169:ASP:HA	1:A:2567:LEU:HD21	1.83	0.60
1:B:3807:LYS:HE2	1:B:3847:PRO:HG3	1.83	0.60
1:A:4432:VAL:HG11	1:A:4470:GLN:HB2	1.84	0.60
1:A:3702:LEU:HD13	1:A:3774:LEU:HD22	1.83	0.60
1:A:3807:LYS:HE2	1:A:3847:PRO:HG3	1.83	0.60
1:A:1789:ASP:HB2	1:A:1865:TYR:HB2	1.82	0.60
1:A:1792:ILE:HB	1:A:1828:LEU:HB3	1.84	0.60
1:A:4198:THR:OG1	1:A:4309:CYS:SG	2.60	0.60
1:A:1443:CYS:O	1:A:1447:CYS:HB2	2.02	0.59
1:B:1341:SER:HB2	1:B:1391:ASN:HD22	1.67	0.59
1:B:4432:VAL:HG11	1:B:4470:GLN:HB2	1.84	0.59
1:B:3228:GLU:HB2	1:B:3265:CYS:HB3	1.84	0.59
1:B:2310:ALA:HB3	1:B:2313:ARG:HE	1.68	0.59
1:B:4198:THR:OG1	1:B:4309:CYS:SG	2.60	0.59
1:B:3702:LEU:HD13	1:B:3774:LEU:HD22	1.83	0.59
1:B:3206:LEU:HD21	1:B:3209:ILE:HD11	1.85	0.59
1:A:3228:GLU:HB2	1:A:3265:CYS:HB3	1.84	0.59
1:A:1341:SER:HB2	1:A:1391:ASN:HD22	1.67	0.58
1:A:2310:ALA:HB3	1:A:2313:ARG:HE	1.68	0.58
1:A:4234:ILE:HG23	1:A:4310:LEU:HD23	1.86	0.58
1:A:3206:LEU:HD21	1:A:3209:ILE:HD11	1.85	0.58
1:B:1443:CYS:O	1:B:1447:CYS:HB2	2.02	0.58
1:B:4234:ILE:HG23	1:B:4310:LEU:HD23	1.86	0.58
1:B:4307:VAL:O	1:B:4311:LEU:HB3	2.04	0.58
1:B:1170:LEU:HD11	1:B:2551:GLN:HG2	1.86	0.58
1:B:1967:GLN:O	1:B:1971:ASN:ND2	2.37	0.58
1:A:1035:PRO:HD2	1:A:1038:LEU:HD12	1.86	0.58
1:A:1170:LEU:HD11	1:A:2551:GLN:HG2	1.86	0.58
1:B:1792:ILE:HB	1:B:1828:LEU:HB3	1.84	0.58
1:A:1967:GLN:O	1:A:1971:ASN:ND2	2.37	0.58
1:A:2308:THR:HG21	1:A:2352:ARG:HH21	1.69	0.57
1:B:4396:VAL:HG13	1:B:4483:LEU:HD13	1.87	0.57
1:A:2703:ARG:HE	1:B:3238:PRO:HB2	1.70	0.56
1:B:1035:PRO:HD2	1:B:1038:LEU:HD12	1.86	0.56
1:A:1534:LEU:HB3	1:A:1537:LEU:HD21	1.87	0.56
1:A:4307:VAL:O	1:A:4311:LEU:HB3	2.04	0.56
1:B:1345:GLY:H	1:B:1348:LYS:HD3	1.70	0.56
1:A:1017:THR:OG1	1:A:1068:GLU:OE2	2.23	0.56
1:A:1014:PHE:HA	1:A:1072:PRO:HD3	1.88	0.56
1:A:1190:GLY:HA3	1:A:1192:LYS:HE3	1.88	0.56
1:A:2809:ARG:O	1:B:2809:ARG:NH2	2.39	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2370:LEU:HD22	1:B:2649:LEU:HD21	1.87	0.56
1:A:2809:ARG:NH2	1:B:2809:ARG:O	2.39	0.56
1:A:4396:VAL:HG13	1:A:4483:LEU:HD13	1.87	0.56
1:B:1014:PHE:HA	1:B:1072:PRO:HD3	1.88	0.56
1:B:1190:GLY:HA3	1:B:1192:LYS:HE3	1.88	0.55
1:A:2370:LEU:HD22	1:A:2649:LEU:HD21	1.87	0.55
1:B:2308:THR:HG21	1:B:2352:ARG:HH21	1.70	0.55
1:B:4420:SER:N	1:B:4423:THR:HG1	2.04	0.55
1:A:2185:ASN:HB2	1:A:2188:SER:HB3	1.88	0.55
1:A:4321:MET:SD	1:A:4322:SER:N	2.76	0.55
1:B:1017:THR:OG1	1:B:1068:GLU:OE2	2.23	0.55
1:B:3239:LEU:HD13	1:B:3255:LEU:HD21	1.89	0.55
1:B:4321:MET:SD	1:B:4322:SER:N	2.76	0.55
1:A:1008:GLU:OE2	1:A:1282:ARG:NH1	2.40	0.55
1:A:2101:ASP:OD1	1:A:2101:ASP:N	2.37	0.55
1:A:3238:PRO:HB2	1:B:2703:ARG:HE	1.70	0.55
1:A:1345:GLY:H	1:A:1348:LYS:HD3	1.70	0.55
1:B:1021:CYS:O	1:B:1056:GLN:NE2	2.40	0.55
1:B:1534:LEU:HB3	1:B:1537:LEU:HD21	1.87	0.55
1:B:2675:ASN:OD1	1:B:2781:ARG:NH1	2.40	0.55
1:A:4420:SER:N	1:A:4423:THR:HG1	2.04	0.55
1:B:1558:ARG:HA	1:B:1762:GLN:HA	1.89	0.55
1:A:1461:ARG:NH2	1:A:2002:GLN:O	2.39	0.55
1:A:2675:ASN:OD1	1:A:2781:ARG:NH1	2.40	0.55
1:B:1008:GLU:OE2	1:B:1282:ARG:NH1	2.40	0.55
1:B:1461:ARG:NH2	1:B:2002:GLN:O	2.39	0.55
1:A:1461:ARG:NH2	1:A:2004:SER:O	2.40	0.54
1:A:1558:ARG:HA	1:A:1762:GLN:HA	1.89	0.54
1:A:1021:CYS:O	1:A:1056:GLN:NE2	2.40	0.54
1:A:2761:ASN:ND2	1:B:2865:SER:O	2.41	0.54
1:A:3239:LEU:HD13	1:A:3255:LEU:HD21	1.89	0.54
1:A:3412:LEU:HD21	1:B:1935:SER:HB2	1.90	0.54
1:A:4154:LEU:HD12	1:A:4155:PRO:HD2	1.90	0.54
1:B:1461:ARG:NH2	1:B:2004:SER:O	2.40	0.54
1:B:1084:PHE:HB2	1:B:1273:LEU:HD22	1.90	0.54
1:B:2185:ASN:HB2	1:B:2188:SER:HB3	1.88	0.54
1:B:3853:SER:HB2	1:B:3966:ALA:HB1	1.90	0.54
1:A:2755:THR:HB	1:A:2817:GLY:H	1.73	0.53
1:B:3345:LEU:HD12	1:B:3382:LEU:HD13	1.91	0.53
1:A:3621:LEU:HD23	1:A:3672:ILE:HG23	1.91	0.53
1:A:1935:SER:HB2	1:B:3412:LEU:HD21	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1799:ALA:HB2	1:A:1849:ARG:HA	1.91	0.53
1:A:2865:SER:O	1:B:2761:ASN:ND2	2.41	0.53
1:A:3345:LEU:HD12	1:A:3382:LEU:HD13	1.91	0.53
1:A:4186:HIS:HB2	1:A:4189:GLN:HG2	1.90	0.53
1:B:1799:ALA:HB2	1:B:1849:ARG:HA	1.91	0.53
1:B:3621:LEU:HD23	1:B:3672:ILE:HG23	1.91	0.53
1:B:4186:HIS:HB2	1:B:4189:GLN:HG2	1.90	0.53
1:A:3797:LEU:O	1:A:3801:LEU:HB3	2.09	0.52
1:B:4154:LEU:HD12	1:B:4155:PRO:HD2	1.90	0.52
1:B:2755:THR:HB	1:B:2817:GLY:H	1.73	0.52
1:B:3797:LEU:O	1:B:3801:LEU:HB3	2.09	0.52
1:A:1084:PHE:HB2	1:A:1273:LEU:HD22	1.90	0.52
1:A:3400:LEU:HD13	1:B:2368:ARG:HG2	1.92	0.52
1:A:4435:TYR:HA	1:A:4438:ARG:HD2	1.92	0.52
1:A:2368:ARG:HG2	1:B:3400:LEU:HD13	1.92	0.52
1:A:3241:THR:OG1	1:B:2763:HIS:ND1	2.43	0.52
1:A:3853:SER:HB2	1:A:3966:ALA:HB1	1.90	0.52
1:A:3550:MET:HE2	1:A:3599:LEU:HG	1.92	0.52
1:B:3433:LYS:HG3	1:B:3502:LEU:HD21	1.92	0.52
1:A:2763:HIS:ND1	1:B:3241:THR:OG1	2.43	0.52
1:B:4435:TYR:HA	1:B:4438:ARG:HD2	1.92	0.52
1:A:3235:ASN:ND2	1:B:2670:PHE:O	2.39	0.52
1:B:3798:PHE:O	1:B:3802:MET:CB	2.57	0.52
1:A:2767:VAL:HG13	1:A:2818:PRO:HB3	1.92	0.51
1:B:1510:ASP:OD1	1:B:1510:ASP:N	2.43	0.51
1:B:3622:VAL:HG23	1:B:3697:LEU:HD22	1.92	0.51
1:A:1030:GLN:HE22	1:A:1047:ALA:HB3	1.76	0.51
1:B:2703:ARG:HH12	1:B:2771:ALA:HB2	1.75	0.51
1:B:3322:HIS:O	1:B:3326:HIS:HB2	2.11	0.51
1:B:2767:VAL:HG13	1:B:2818:PRO:HB3	1.92	0.51
1:A:2049:PHE:HE1	1:A:2085:VAL:HG11	1.76	0.51
1:A:2674:ALA:O	1:A:2717:ASN:ND2	2.41	0.51
1:A:2703:ARG:HH12	1:A:2771:ALA:HB2	1.75	0.51
1:A:3622:VAL:HG23	1:A:3697:LEU:HD22	1.92	0.51
1:A:3415:ASP:HA	1:A:3418:ILE:HD12	1.93	0.51
1:A:3433:LYS:HG3	1:A:3502:LEU:HD21	1.92	0.51
1:B:1030:GLN:HE22	1:B:1047:ALA:HB3	1.75	0.51
1:A:3322:HIS:O	1:A:3326:HIS:HB2	2.11	0.50
1:B:3415:ASP:HA	1:B:3418:ILE:HD12	1.93	0.50
1:A:3401:ASN:OD1	1:B:2368:ARG:NH2	2.45	0.50
1:B:2101:ASP:OD1	1:B:2101:ASP:N	2.37	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1309:LEU:HD21	1:A:1357:LYS:HB3	1.94	0.50
1:B:2125:LEU:HB3	1:B:2317:VAL:HG21	1.93	0.50
1:B:3389:ASN:HA	1:B:3410:ASN:HD21	1.76	0.50
1:A:1454:VAL:HG13	1:A:2009:LEU:HD22	1.94	0.50
1:B:3550:MET:HE2	1:B:3599:LEU:HG	1.92	0.50
1:B:4062:ALA:HB1	1:B:4158:ALA:HB1	1.94	0.50
1:A:3604:GLN:NE2	1:A:3678:GLU:O	2.45	0.50
1:A:4226:LEU:HD11	1:A:4347:LEU:HD23	1.94	0.50
1:B:1296:CYS:O	1:B:1300:GLN:HB2	2.12	0.50
1:A:3389:ASN:HA	1:A:3410:ASN:HD21	1.76	0.50
1:B:2049:PHE:HE1	1:B:2085:VAL:HG11	1.76	0.50
1:B:1790:VAL:HB	1:B:1830:LEU:HB2	1.93	0.49
1:A:1296:CYS:O	1:A:1300:GLN:HB2	2.12	0.49
1:B:4226:LEU:HD11	1:B:4347:LEU:HD23	1.94	0.49
1:A:2701:LEU:HD12	1:B:2862:LYS:HE2	1.95	0.49
1:A:4231:LEU:HA	1:A:4234:ILE:HD12	1.95	0.49
1:A:1010:LEU:HD13	1:A:1280:ILE:HG22	1.94	0.49
1:B:3210:HIS:HB2	1:B:3283:LYS:HB2	1.95	0.49
1:A:2125:LEU:HB3	1:A:2317:VAL:HG21	1.93	0.49
1:A:2368:ARG:NH2	1:B:3401:ASN:OD1	2.45	0.49
1:A:2861:ASP:OD1	1:A:2861:ASP:N	2.45	0.49
1:B:1309:LEU:HD21	1:B:1357:LYS:HB3	1.94	0.49
1:B:1466:GLU:HA	1:B:1469:LEU:HD12	1.94	0.49
1:B:2051:HIS:O	1:B:2055:SER:OG	2.31	0.49
1:B:2107:LEU:HA	1:B:2110:ILE:HG22	1.94	0.49
1:A:3210:HIS:HB2	1:A:3283:LYS:HB2	1.95	0.49
1:B:1010:LEU:HD13	1:B:1280:ILE:HG22	1.94	0.49
1:A:2862:LYS:HE2	1:B:2701:LEU:HD12	1.95	0.49
1:A:3848:VAL:HA	1:A:3970:LEU:HB2	1.95	0.49
1:A:2563:GLN:OE1	1:A:2564:GLN:NE2	2.46	0.49
1:A:4062:ALA:HB1	1:A:4158:ALA:HB1	1.94	0.49
1:A:2739:VAL:HG13	1:A:2797:LEU:HD22	1.94	0.49
1:B:2861:ASP:OD1	1:B:2861:ASP:N	2.45	0.49
1:B:4231:LEU:HA	1:B:4234:ILE:HD12	1.94	0.49
1:A:3346:GLN:HB3	1:A:3405:LEU:HG	1.95	0.48
1:A:1790:VAL:HB	1:A:1830:LEU:HB2	1.93	0.48
1:B:4347:LEU:HA	1:B:4350:LEU:HG	1.96	0.48
1:A:1466:GLU:HA	1:A:1469:LEU:HD12	1.94	0.48
1:A:1471:THR:HG21	1:A:2097:ILE:HG22	1.95	0.48
1:A:2051:HIS:O	1:A:2055:SER:OG	2.31	0.48
1:B:2563:GLN:OE1	1:B:2564:GLN:NE2	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1909:ASP:OD2	1:A:1913:ARG:NH1	2.47	0.48
1:B:1454:VAL:HG13	1:B:2009:LEU:HD22	1.94	0.48
1:B:1471:THR:HG21	1:B:2097:ILE:HG22	1.95	0.48
1:B:1909:ASP:OD2	1:B:1913:ARG:NH1	2.47	0.48
1:B:2739:VAL:HG13	1:B:2797:LEU:HD22	1.94	0.48
1:B:3814:SER:HB2	1:B:3993:VAL:HB	1.95	0.48
1:A:3798:PHE:O	1:A:3802:MET:CB	2.57	0.48
1:A:1383:ARG:NH1	1:A:2566:GLU:OE1	2.47	0.48
1:A:3060:THR:O	1:B:2380:ARG:NH1	2.46	0.48
1:B:1383:ARG:NH1	1:B:2566:GLU:OE1	2.47	0.47
1:B:3346:GLN:HB3	1:B:3405:LEU:HG	1.95	0.47
1:B:1551:SER:O	1:B:1555:ARG:NH1	2.48	0.47
1:B:3604:GLN:NE2	1:B:3678:GLU:O	2.45	0.47
1:A:2380:ARG:NH1	1:B:3060:THR:O	2.47	0.47
1:B:2129:ASP:HB3	1:B:2317:VAL:HG22	1.97	0.47
1:A:3174:PRO:HG2	1:A:3280:SER:HB3	1.95	0.47
1:B:1786:LEU:HD21	1:B:1874:GLU:HB3	1.97	0.47
1:A:3218:LEU:HB2	1:B:3218:LEU:HB2	1.95	0.47
1:B:1058:ASP:OD2	1:B:1058:ASP:N	2.48	0.47
1:A:1551:SER:O	1:A:1555:ARG:NH1	2.47	0.47
1:A:1786:LEU:HD21	1:A:1874:GLU:HB3	1.97	0.47
1:A:2107:LEU:HA	1:A:2110:ILE:HG22	1.94	0.47
1:B:3812:LEU:HD22	1:B:3859:VAL:HG11	1.96	0.47
1:A:3812:LEU:HD22	1:A:3859:VAL:HG11	1.96	0.47
1:A:4347:LEU:HA	1:A:4350:LEU:HG	1.96	0.47
1:B:3848:VAL:HA	1:B:3970:LEU:HB2	1.95	0.47
1:A:3760:HIS:HD2	1:A:3985:GLY:HA3	1.79	0.47
1:B:3174:PRO:HG2	1:B:3280:SER:HB3	1.95	0.47
1:A:2670:PHE:O	1:B:3235:ASN:ND2	2.39	0.47
1:A:3520:CYS:HA	1:A:3525:LYS:HD3	1.96	0.47
1:B:3520:CYS:HA	1:B:3525:LYS:HD3	1.96	0.47
1:B:3775:PHE:O	1:B:4073:ARG:NH1	2.47	0.47
1:A:2842:ILE:HG23	1:A:2915:LEU:HD13	1.97	0.46
1:A:3775:PHE:O	1:A:4073:ARG:NH1	2.47	0.46
1:A:3814:SER:HB2	1:A:3993:VAL:HB	1.96	0.46
1:A:1911:GLN:HG3	1:A:1970:LEU:HD11	1.98	0.46
1:B:1096:ILE:HA	1:B:1202:ALA:HA	1.98	0.46
1:B:3760:HIS:HD2	1:B:3985:GLY:HA3	1.79	0.46
1:A:1924:LEU:O	1:A:1927:SER:OG	2.33	0.46
1:A:2129:ASP:HB3	1:A:2317:VAL:HG22	1.97	0.46
1:A:2553:LEU:HD23	1:A:2567:LEU:HD13	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1327:SER:HG	1:B:1380:LYS:HZ2	1.59	0.46
1:B:3629:CYS:HA	1:B:3704:LEU:HD13	1.98	0.46
1:B:2837:VAL:HG13	1:B:2842:ILE:HD11	1.97	0.46
1:B:1081:ASP:HB2	1:B:1279:THR:HB	1.98	0.46
1:A:2837:VAL:HG13	1:A:2842:ILE:HD11	1.97	0.46
1:B:1911:GLN:HG3	1:B:1970:LEU:HD11	1.98	0.46
1:B:2842:ILE:HG23	1:B:2915:LEU:HD13	1.97	0.46
1:A:2153:MET:HE3	1:A:2153:MET:HB3	1.70	0.46
1:B:4172:LEU:HA	1:B:4175:VAL:HG12	1.98	0.46
1:B:1045:ASP:HA	1:B:1048:GLN:HG3	1.98	0.46
1:A:1045:ASP:HA	1:A:1048:GLN:HG3	1.98	0.45
1:A:1046:ALA:HA	1:A:1049:HIS:CD2	2.51	0.45
1:A:4172:LEU:HA	1:A:4175:VAL:HG12	1.98	0.45
1:B:1076:MET:SD	1:B:1076:MET:N	2.87	0.45
1:A:2129:ASP:O	1:A:2320:LYS:NZ	2.42	0.45
1:A:3802:MET:HG3	1:A:4058:LEU:HD13	1.98	0.45
1:A:1096:ILE:HA	1:A:1202:ALA:HA	1.98	0.45
1:B:1153:HIS:HB3	1:B:1156:ASP:HB2	1.98	0.45
1:B:2034:ALA:O	1:B:2038:SER:OG	2.32	0.45
1:A:1081:ASP:HB2	1:A:1279:THR:HB	1.98	0.45
1:A:1014:PHE:HE1	1:A:1069:LEU:HD22	1.81	0.45
1:B:1046:ALA:HA	1:B:1049:HIS:CD2	2.51	0.45
1:B:1298:MET:HE3	1:B:1298:MET:HB2	1.76	0.45
1:A:1298:MET:HE3	1:A:1298:MET:HB2	1.76	0.45
1:A:3222:PRO:HG3	1:A:3268:LEU:HD23	1.99	0.45
1:B:1534:LEU:HD23	1:B:1791:LEU:HD13	1.98	0.45
1:A:3515:SER:O	1:A:3525:LYS:NZ	2.44	0.45
1:B:68:VAL:O	1:B:77:LEU:N	2.45	0.45
1:B:1095:GLN:O	1:B:1203:VAL:N	2.50	0.45
1:A:1153:HIS:HB3	1:A:1156:ASP:HB2	1.98	0.45
1:A:1534:LEU:HD23	1:A:1791:LEU:HD13	1.98	0.45
1:B:2553:LEU:HD23	1:B:2567:LEU:HD13	1.97	0.45
1:A:1095:GLN:O	1:A:1203:VAL:N	2.49	0.45
1:A:3629:CYS:HA	1:A:3704:LEU:HD13	1.98	0.45
1:B:2674:ALA:O	1:B:2717:ASN:ND2	2.41	0.45
1:B:3802:MET:HG3	1:B:4058:LEU:HD13	1.98	0.45
1:A:3187:PHE:HE2	1:A:3277:LEU:HB2	1.83	0.44
1:A:3485:ALA:HB1	1:A:3836:GLY:HA2	2.00	0.44
1:A:4360:MET:HE1	1:A:4386:LEU:HD21	2.00	0.44
1:B:2153:MET:HE3	1:B:2153:MET:HB3	1.70	0.44
1:B:2557:LEU:HD21	1:B:2566:GLU:HB3	1.99	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4307:VAL:O	1:B:4311:LEU:CB	2.65	0.44
1:B:4399:LEU:HB2	1:B:4421:VAL:HB	1.99	0.44
1:A:1779:LEU:HD21	1:A:1861:LEU:HD11	2.00	0.44
1:A:4307:VAL:O	1:A:4311:LEU:CB	2.65	0.44
1:B:3485:ALA:HB1	1:B:3836:GLY:HA2	1.99	0.44
1:B:3844:LEU:HD13	1:B:3858:ARG:HD2	2.00	0.44
1:A:2322:VAL:HG21	1:A:2360:ILE:HG12	2.00	0.44
1:B:3222:PRO:HG3	1:B:3268:LEU:HD23	1.99	0.44
1:A:1023:VAL:HG13	1:A:1056:GLN:HE22	1.82	0.44
1:A:3844:LEU:HD13	1:A:3858:ARG:HD2	1.99	0.44
1:B:1014:PHE:HE1	1:B:1069:LEU:HD22	1.81	0.44
1:B:1101:LEU:HB2	1:B:1197:LEU:HB2	1.99	0.44
1:B:3359:MET:HE2	1:B:3364:ILE:HD13	1.99	0.44
1:A:3147:HIS:HE1	1:A:3293:THR:O	2.01	0.44
1:B:1779:LEU:HD21	1:B:1861:LEU:HD11	2.00	0.44
1:B:4059:GLN:HA	1:B:4162:LEU:HD21	1.99	0.44
1:A:4059:GLN:HA	1:A:4162:LEU:HD21	1.99	0.44
1:A:4399:LEU:HB2	1:A:4421:VAL:HB	1.99	0.44
1:B:1023:VAL:HG13	1:B:1056:GLN:HE22	1.82	0.44
1:B:3187:PHE:HE2	1:B:3277:LEU:HB2	1.83	0.44
1:B:4205:ARG:HG3	1:B:4312:GLN:HB3	1.99	0.44
1:A:2318:VAL:HG13	1:A:2344:LEU:HG	2.00	0.44
1:A:2557:LEU:HD21	1:A:2566:GLU:HB3	1.99	0.43
1:A:3359:MET:HE2	1:A:3364:ILE:HD13	1.99	0.43
1:B:3754:LEU:O	1:B:3758:SER:OG	2.34	0.43
1:A:2632:LEU:HD22	1:A:2641:VAL:HG11	2.00	0.43
1:B:1771:SER:OG	1:B:1849:ARG:O	2.33	0.43
1:B:2082:LEU:HD12	1:B:2082:LEU:HA	1.84	0.43
1:A:1101:LEU:HB2	1:A:1197:LEU:HB2	1.99	0.43
1:A:1472:ARG:HD2	1:A:1930:LEU:HD13	2.01	0.43
1:A:4205:ARG:HG3	1:A:4312:GLN:HB3	1.99	0.43
1:B:988:LEU:HD12	1:B:997:ILE:HG23	2.00	0.43
1:A:1090:ILE:HD13	1:A:1272:LEU:HD21	2.00	0.43
1:B:2322:VAL:HG21	1:B:2360:ILE:HG12	2.00	0.43
1:A:2783:GLN:HG3	1:A:2832:GLN:HE22	1.84	0.43
1:A:2798:LEU:HD13	1:A:2829:THR:HG22	2.00	0.43
1:B:2798:LEU:HD13	1:B:2829:THR:HG22	2.01	0.43
1:B:3352:LEU:HD11	1:B:3416:SER:HB3	2.00	0.43
1:A:2853:VAL:HG11	1:A:2909:LEU:HD21	2.01	0.43
1:B:3110:SER:OG	1:B:3111:MET:N	2.46	0.43
1:B:4360:MET:HE1	1:B:4386:LEU:HD21	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1515:LEU:HD11	1:B:2062:LEU:HD21	2.00	0.43
1:B:1090:ILE:HD13	1:B:1272:LEU:HD21	2.00	0.43
1:B:1472:ARG:HD2	1:B:1930:LEU:HD13	2.01	0.43
1:B:2713:THR:O	1:B:2716:THR:OG1	2.31	0.43
1:B:2783:GLN:HG3	1:B:2832:GLN:HE22	1.84	0.43
1:A:68:VAL:O	1:A:77:LEU:N	2.45	0.43
1:A:3846:LEU:HD13	1:A:3850:THR:HG21	2.01	0.43
1:A:3051:TYR:CD1	1:A:3052:MET:HG2	2.54	0.42
1:A:1510:ASP:N	1:A:1510:ASP:OD1	2.43	0.42
1:B:2632:LEU:HD22	1:B:2641:VAL:HG11	2.00	0.42
1:A:1803:ILE:HG22	1:A:1818:VAL:HG12	2.01	0.42
1:B:3147:HIS:HE1	1:B:3293:THR:O	2.01	0.42
1:B:3552:ILE:HG21	1:B:3617:LEU:HD12	2.01	0.42
1:A:1194:ARG:HA	1:A:1194:ARG:HD3	1.88	0.42
1:A:3352:LEU:HD11	1:A:3416:SER:HB3	2.00	0.42
1:B:140:LEU:O	1:B:194:VAL:N	2.44	0.42
1:B:2318:VAL:HG13	1:B:2344:LEU:HG	2.00	0.42
1:B:3051:TYR:CD1	1:B:3052:MET:HG2	2.54	0.42
1:B:2021:LEU:HD13	1:B:2584:LEU:HD21	2.01	0.42
1:B:2311:HIS:HE1	1:B:2355:ILE:HG23	1.84	0.42
1:B:3116:MET:HB2	1:B:3116:MET:HE2	1.68	0.42
1:A:1487:LEU:HD22	1:A:1968:LEU:HD11	2.02	0.42
1:A:2135:LEU:HD12	1:A:2135:LEU:HA	1.91	0.42
1:B:1479:PRO:O	1:B:1914:TYR:OH	2.34	0.42
1:A:1515:LEU:HD11	1:A:2062:LEU:HD21	2.00	0.42
1:B:1924:LEU:O	1:B:1927:SER:OG	2.33	0.42
1:B:3146:ILE:HG13	1:B:3285:LEU:HD23	2.02	0.42
1:A:140:LEU:O	1:A:194:VAL:N	2.43	0.42
1:A:3146:ILE:HG13	1:A:3285:LEU:HD23	2.02	0.42
1:A:3552:ILE:HG21	1:A:3617:LEU:HD12	2.01	0.42
1:A:1083:LYS:HB2	1:A:1277:SER:HB2	2.02	0.42
1:A:1158:LEU:HD12	1:A:1184:LEU:HA	2.02	0.42
1:A:2034:ALA:O	1:A:2038:SER:OG	2.32	0.42
1:B:1487:LEU:HD22	1:B:1968:LEU:HD11	2.02	0.42
1:B:1803:ILE:HG22	1:B:1818:VAL:HG12	2.01	0.42
1:B:3701:LEU:HD13	1:B:3749:THR:HG23	2.01	0.42
1:A:988:LEU:HD12	1:A:997:ILE:HG23	2.00	0.42
1:A:1371:PHE:HE2	1:A:1416:LEU:HA	1.85	0.42
1:B:1542:PRO:HB2	1:B:1759:PRO:HD3	2.02	0.42
1:B:3846:LEU:HD13	1:B:3850:THR:HG21	2.01	0.42
1:A:2311:HIS:HE1	1:A:2355:ILE:HG23	1.84	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1415:PHE:HB3	1:A:1991:LEU:HD23	2.02	0.41
1:A:2021:LEU:HD13	1:A:2584:LEU:HD21	2.02	0.41
1:A:4211:THR:HG21	1:A:4221:LEU:HD23	2.02	0.41
1:B:135:VAL:HA	1:B:199:PRO:HA	2.02	0.41
1:B:1371:PHE:HE2	1:B:1416:LEU:HA	1.85	0.41
1:B:2795:SER:HB3	1:B:2834:PHE:HD1	1.85	0.41
1:B:4211:THR:HG21	1:B:4221:LEU:HD23	2.02	0.41
1:A:1542:PRO:HB2	1:A:1759:PRO:HD3	2.02	0.41
1:A:2082:LEU:HD12	1:A:2082:LEU:HA	1.84	0.41
1:A:2795:SER:HB3	1:A:2834:PHE:HD1	1.84	0.41
1:B:2853:VAL:HG11	1:B:2909:LEU:HD21	2.01	0.41
1:A:135:VAL:HA	1:A:199:PRO:HA	2.02	0.41
1:A:1943:LEU:HG	1:B:3114:THR:HG22	2.03	0.41
1:A:3318:ARG:HG2	1:A:3359:MET:SD	2.61	0.41
1:A:3757:ILE:HD13	1:A:3767:MET:HE2	2.03	0.41
1:B:1083:LYS:HB2	1:B:1277:SER:HB2	2.02	0.41
1:B:2554:ASP:N	1:B:2554:ASP:OD1	2.53	0.41
1:A:2151:ILE:HD13	1:A:2151:ILE:HA	1.91	0.41
1:A:4167:HIS:HB3	1:A:4199:LEU:HD21	2.02	0.41
1:A:4377:PRO:HA	1:A:4380:ARG:HE	1.86	0.41
1:B:1443:CYS:O	1:B:1447:CYS:CB	2.69	0.41
1:B:3797:LEU:O	1:B:3801:LEU:CB	2.68	0.41
1:B:1148:PRO:HA	1:B:1151:GLU:HB3	2.02	0.41
1:B:4432:VAL:HG13	1:B:4466:VAL:HG12	2.03	0.41
1:B:4436:THR:HA	1:B:4439:LEU:HG	2.03	0.41
1:A:998:LEU:HB3	1:A:1328:LEU:HB3	2.02	0.41
1:A:1029:GLN:HG3	1:A:1033:ARG:HE	1.86	0.41
1:A:1916:LEU:HD23	1:B:3800:GLN:HE21	1.85	0.41
1:A:4238:LEU:HD13	1:A:4356:LEU:HD13	2.03	0.41
1:B:2655:LEU:HD23	1:B:2655:LEU:HA	1.93	0.41
1:B:2826:LEU:HD23	1:B:2826:LEU:HA	1.91	0.41
1:B:3445:ASP:HB3	1:B:3472:LEU:HD13	2.03	0.41
1:A:1011:THR:O	1:A:1049:HIS:ND1	2.54	0.41
1:A:2036:LEU:HD23	1:A:2071:LEU:HD13	2.03	0.41
1:A:3330:LEU:O	1:A:3334:MET:HG2	2.21	0.41
1:A:3701:LEU:HD13	1:A:3749:THR:HG23	2.01	0.41
1:B:998:LEU:HB3	1:B:1328:LEU:HB3	2.02	0.41
1:B:1433:ASN:HA	1:B:1436:LYS:HZ3	1.85	0.41
1:B:3685:MET:HE2	1:B:3685:MET:HB2	1.99	0.41
1:A:4357:ILE:HA	1:A:4360:MET:HG3	2.03	0.41
1:B:2854:HIS:O	1:B:2858:THR:OG1	2.33	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1148:PRO:HA	1:A:1151:GLU:HB3	2.02	0.40
1:A:3800:GLN:HE21	1:B:1916:LEU:HD23	1.85	0.40
1:A:1511:LEU:HD12	1:A:2105:MET:HB3	2.04	0.40
1:A:2554:ASP:OD1	1:A:2554:ASP:N	2.53	0.40
1:A:2702:LEU:HG	1:A:2703:ARG:NH1	2.37	0.40
1:A:3797:LEU:O	1:A:3801:LEU:CB	2.68	0.40
1:B:1014:PHE:CE1	1:B:1069:LEU:HD22	2.56	0.40
1:B:1415:PHE:HB3	1:B:1991:LEU:HD23	2.02	0.40
1:B:2702:LEU:HG	1:B:2703:ARG:NH1	2.37	0.40
1:A:1380:LYS:HE2	1:A:1834:ILE:HG23	2.03	0.40
1:A:3112:VAL:HG13	1:B:2159:MET:HE2	2.02	0.40
1:A:3114:THR:HG22	1:B:1943:LEU:HG	2.03	0.40
1:A:3599:LEU:HD23	1:A:3599:LEU:HA	1.98	0.40
1:A:3807:LYS:HA	1:A:3847:PRO:HA	2.03	0.40
1:B:1186:LYS:C	1:B:1292:ARG:HH22	2.29	0.40
1:B:1194:ARG:HA	1:B:1194:ARG:HD3	1.88	0.40
1:B:1380:LYS:HE2	1:B:1834:ILE:HG23	2.03	0.40
1:B:3613:LEU:HD23	1:B:3613:LEU:HA	1.95	0.40
1:A:4436:THR:HA	1:A:4439:LEU:HG	2.03	0.40
1:B:1158:LEU:HD12	1:B:1184:LEU:HA	2.02	0.40
1:B:1357:LYS:HA	1:B:1360:LYS:HD2	2.03	0.40
1:B:2651:LEU:HD21	1:B:2711:SER:HA	2.04	0.40
1:B:3318:ARG:HG2	1:B:3359:MET:SD	2.60	0.40
1:B:1043:HIS:CE1	1:B:1815:ARG:HA	2.57	0.40
1:B:2373:LEU:HD23	1:B:2373:LEU:HA	1.96	0.40
1:B:3757:ILE:HD13	1:B:3767:MET:HE2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	2841/4896 (58%)	2786 (98%)	55 (2%)	0	100	100
1	B	2841/4896 (58%)	2787 (98%)	54 (2%)	0	100	100
All	All	5682/9792 (58%)	5573 (98%)	109 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	2046/4236 (48%)	2046 (100%)	0	100	100
1	B	2046/4236 (48%)	2046 (100%)	0	100	100
All	All	4092/8472 (48%)	4092 (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 (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1040	GLN
1	A	1056	GLN
1	A	1305	HIS
1	A	1961	GLN
1	A	2136	GLN
1	A	2311	HIS
1	A	2399	GLN
1	A	2975	GLN
1	A	3041	GLN
1	A	3147	HIS
1	A	3428	GLN
1	A	3513	ASN
1	A	3660	ASN
1	A	3747	ASN
1	A	3962	GLN
1	A	4169	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	1040	GLN
1	B	1056	GLN
1	B	1305	HIS
1	B	1961	GLN
1	B	2037	GLN
1	B	2311	HIS
1	B	2399	GLN
1	B	2975	GLN
1	B	3095	ASN
1	B	3147	HIS
1	B	3428	GLN
1	B	3513	ASN
1	B	3660	ASN
1	B	4169	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

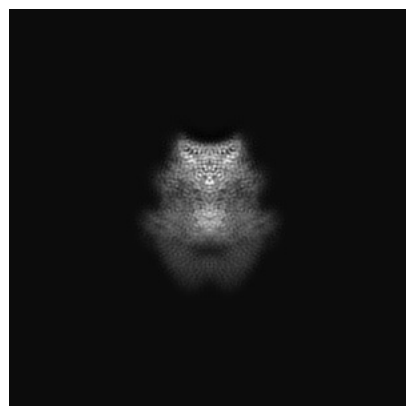
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-35759. These allow visual inspection of the internal detail of the map and identification of artifacts.

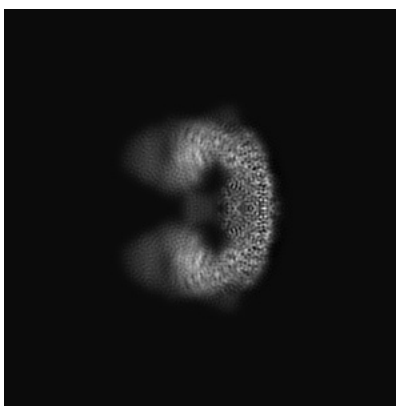
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

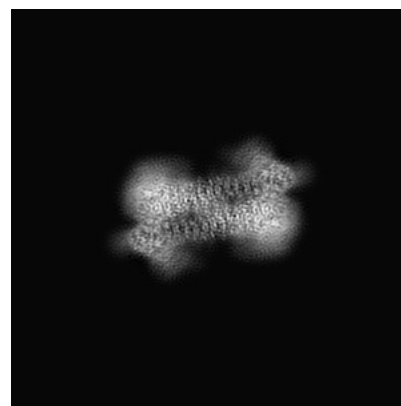
6.1.1 Primary map



X

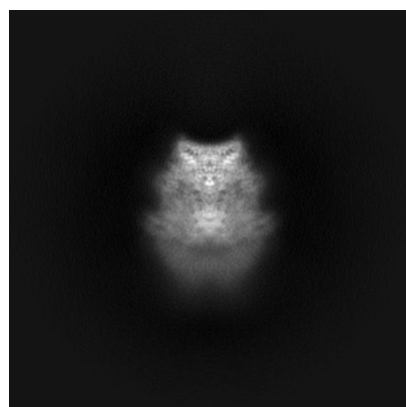


Y

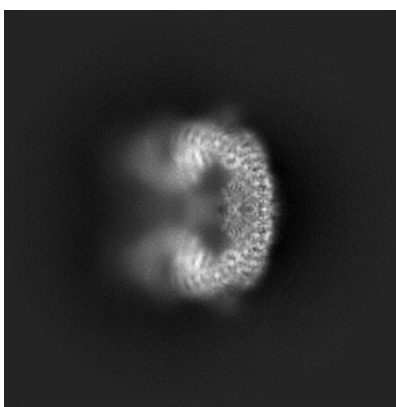


Z

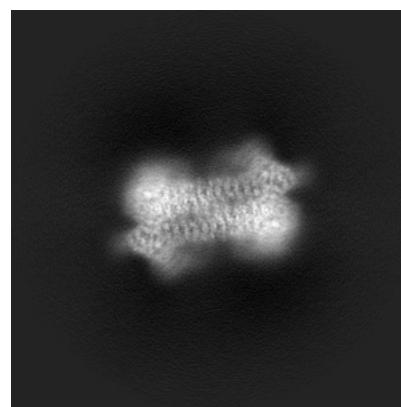
6.1.2 Raw map



X



Y



Z

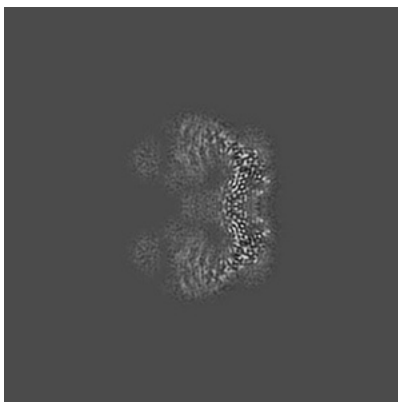
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

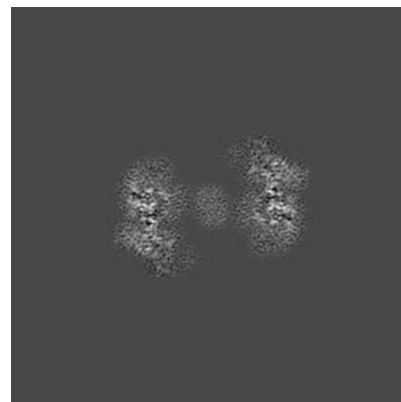
6.2.1 Primary map



X Index: 160

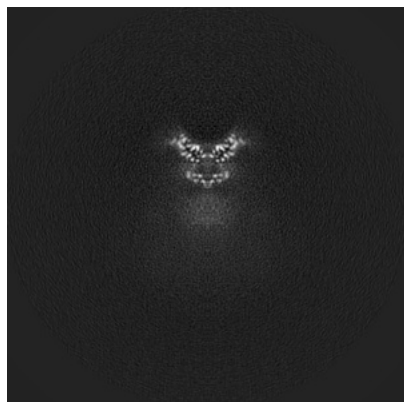


Y Index: 160

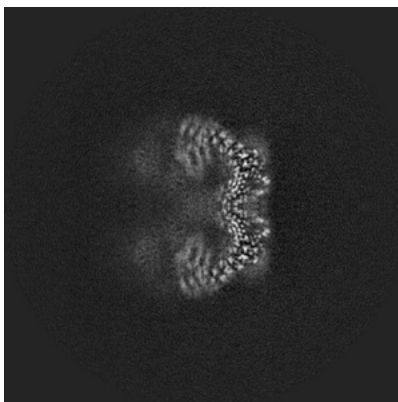


Z Index: 160

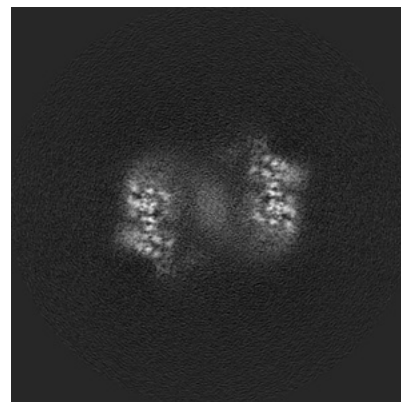
6.2.2 Raw map



X Index: 160



Y Index: 160

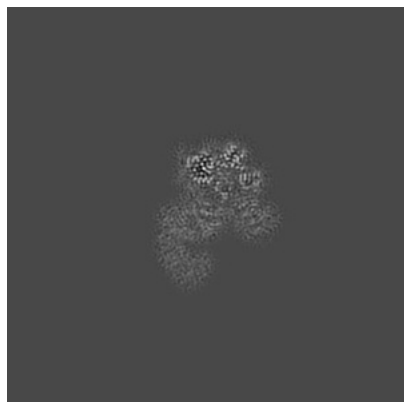


Z Index: 160

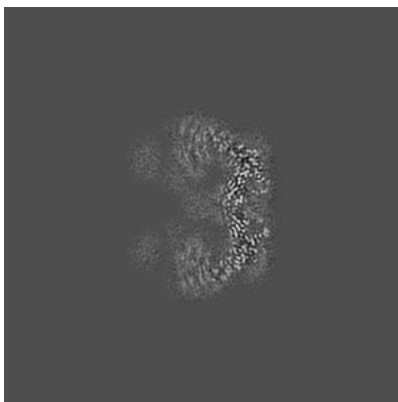
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

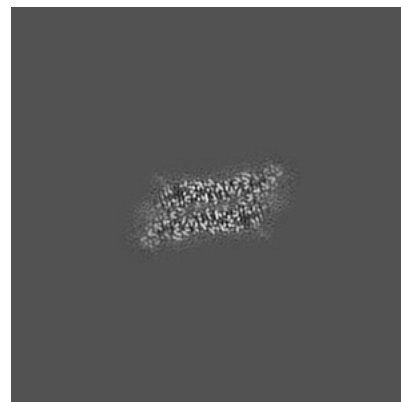
6.3.1 Primary map



X Index: 202

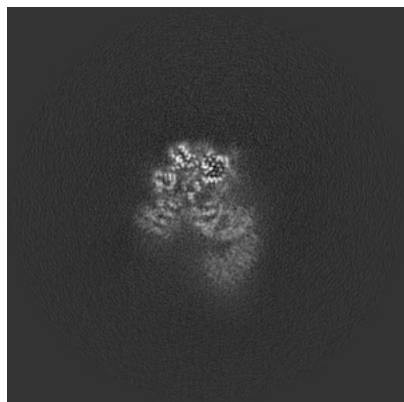


Y Index: 159

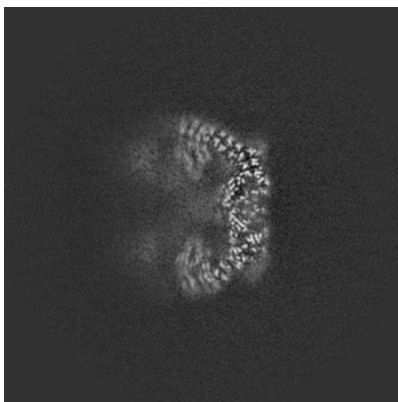


Z Index: 202

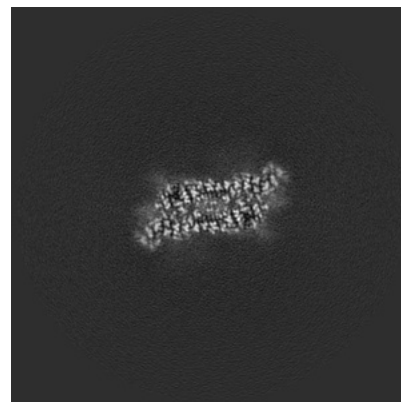
6.3.2 Raw map



X Index: 118



Y Index: 158

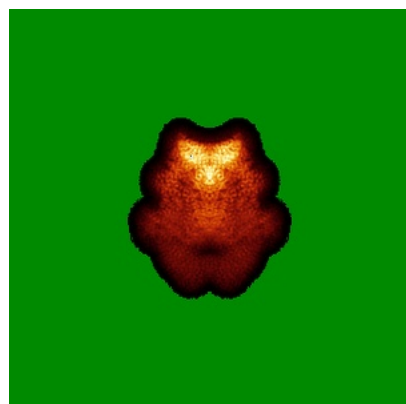


Z Index: 201

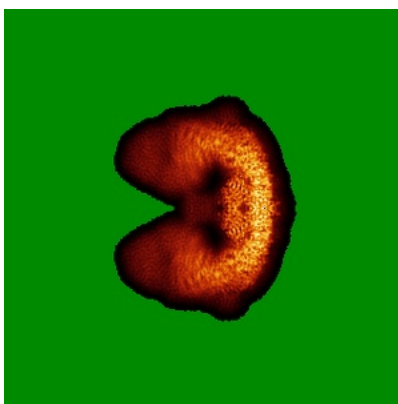
The images above show the largest variance slices of the map in three orthogonal directions.

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

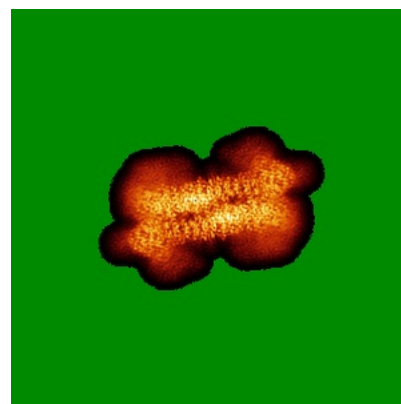
6.4.1 Primary map



X

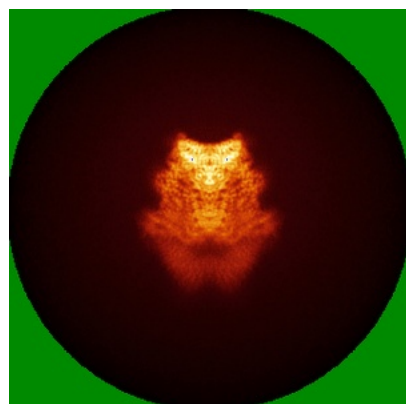


Y

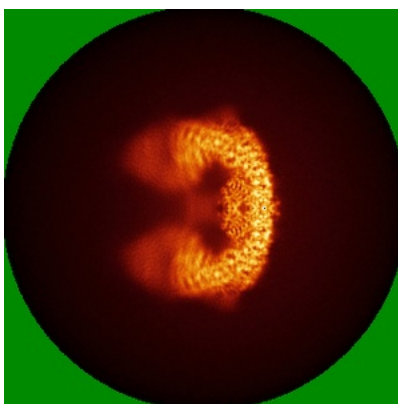


Z

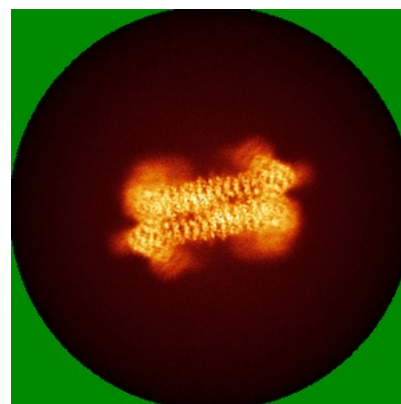
6.4.2 Raw map



X



Y

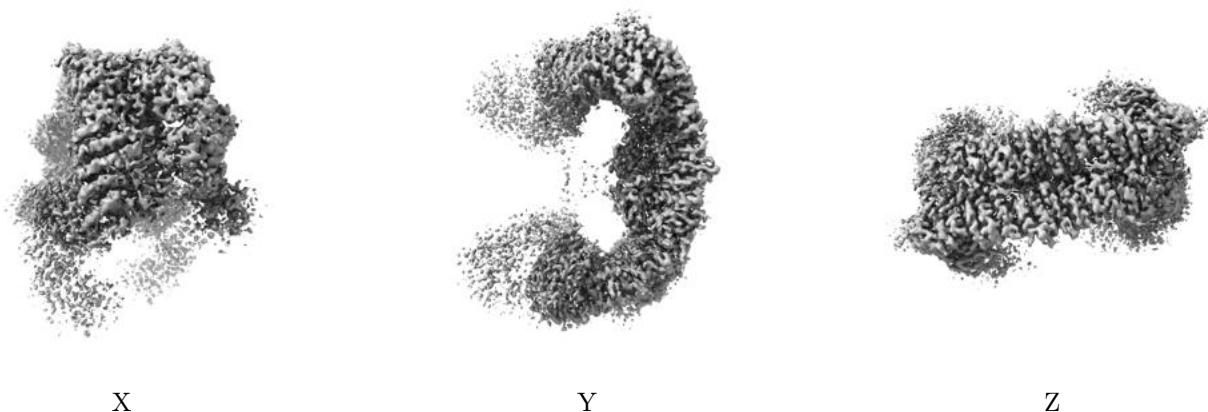


Z

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 0.03. 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.

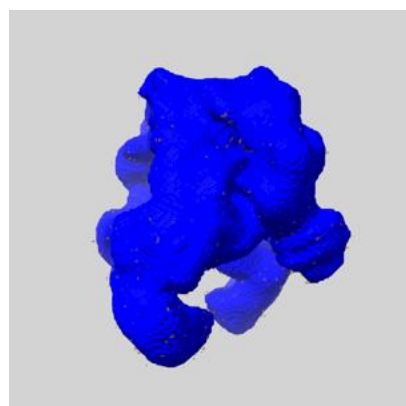
6.6 Mask visualisation [i](#)

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

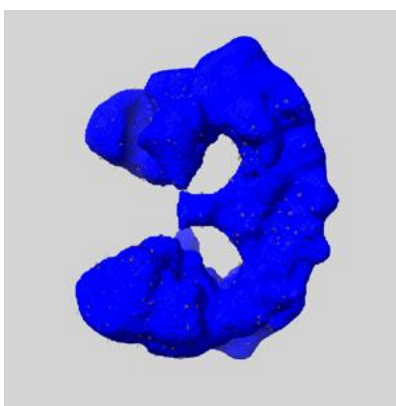
A mask typically either:

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

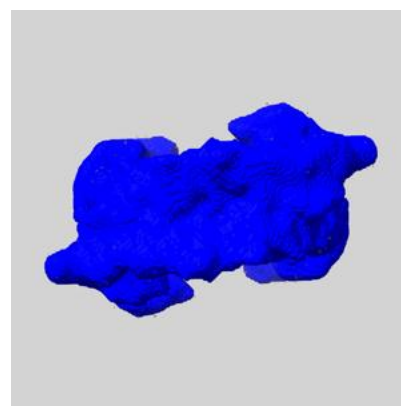
6.6.1 emd_35759_msk_1.map [i](#)



X



Y

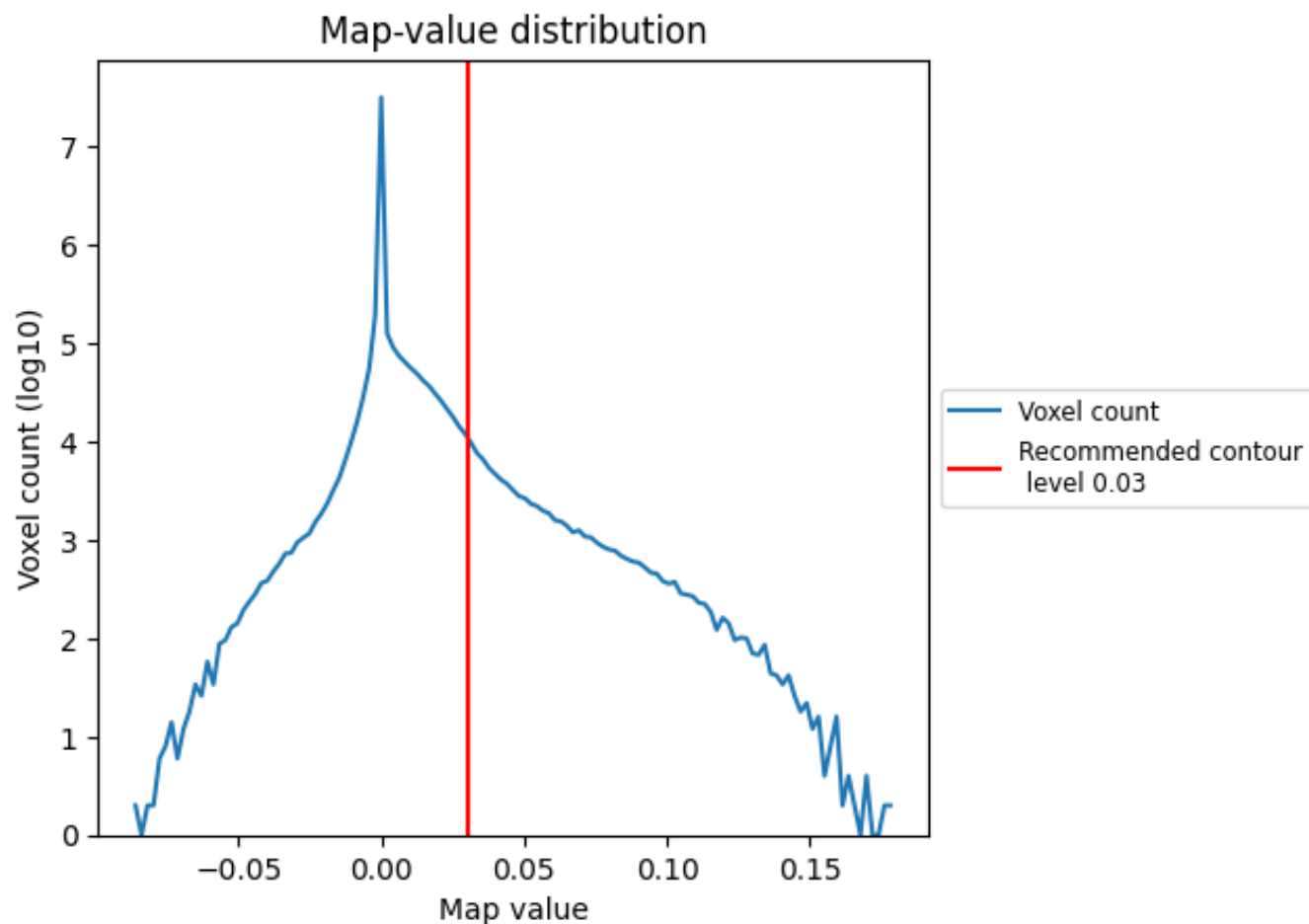


Z

7 Map analysis [i](#)

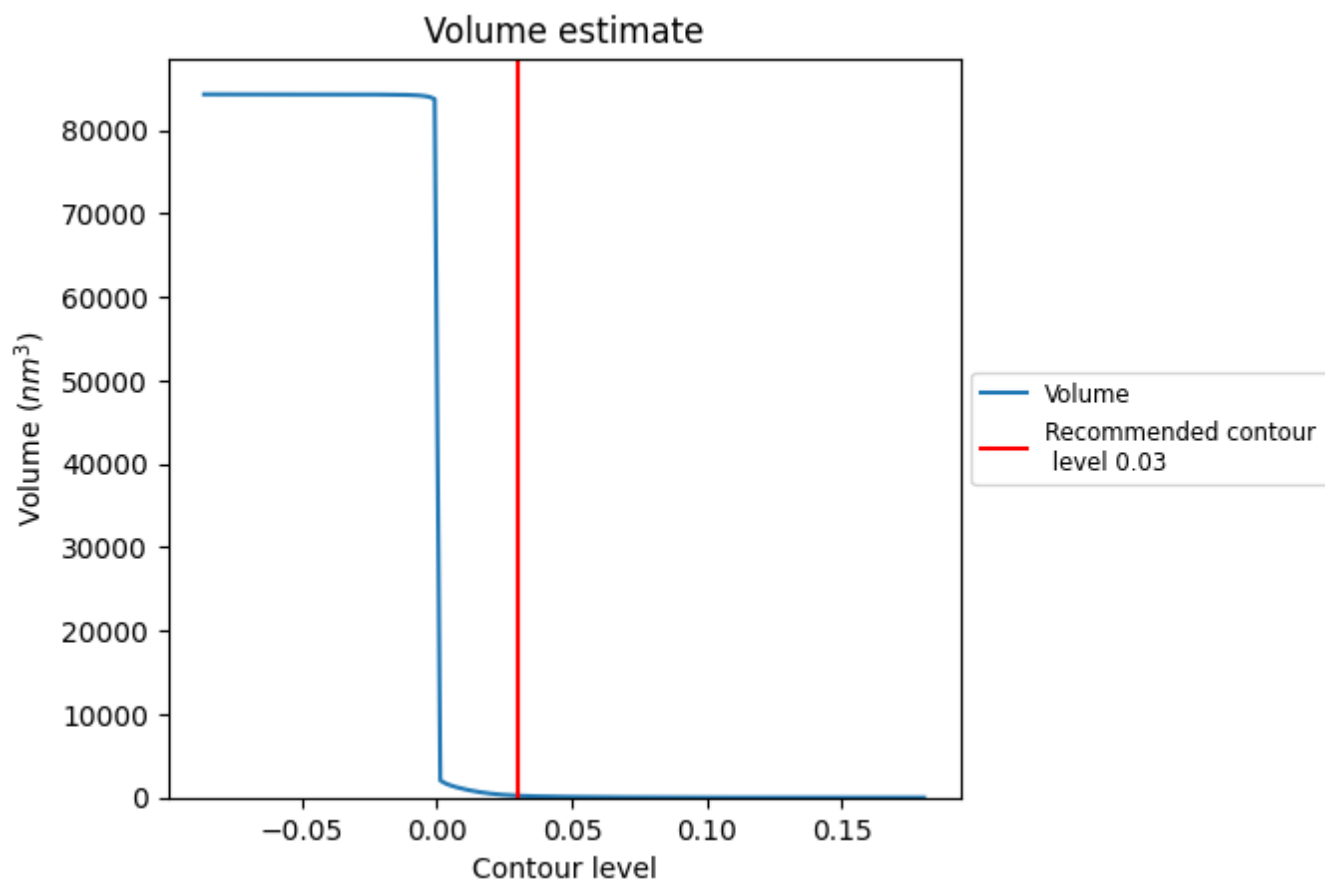
This section contains the results of statistical analysis of the map.

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.

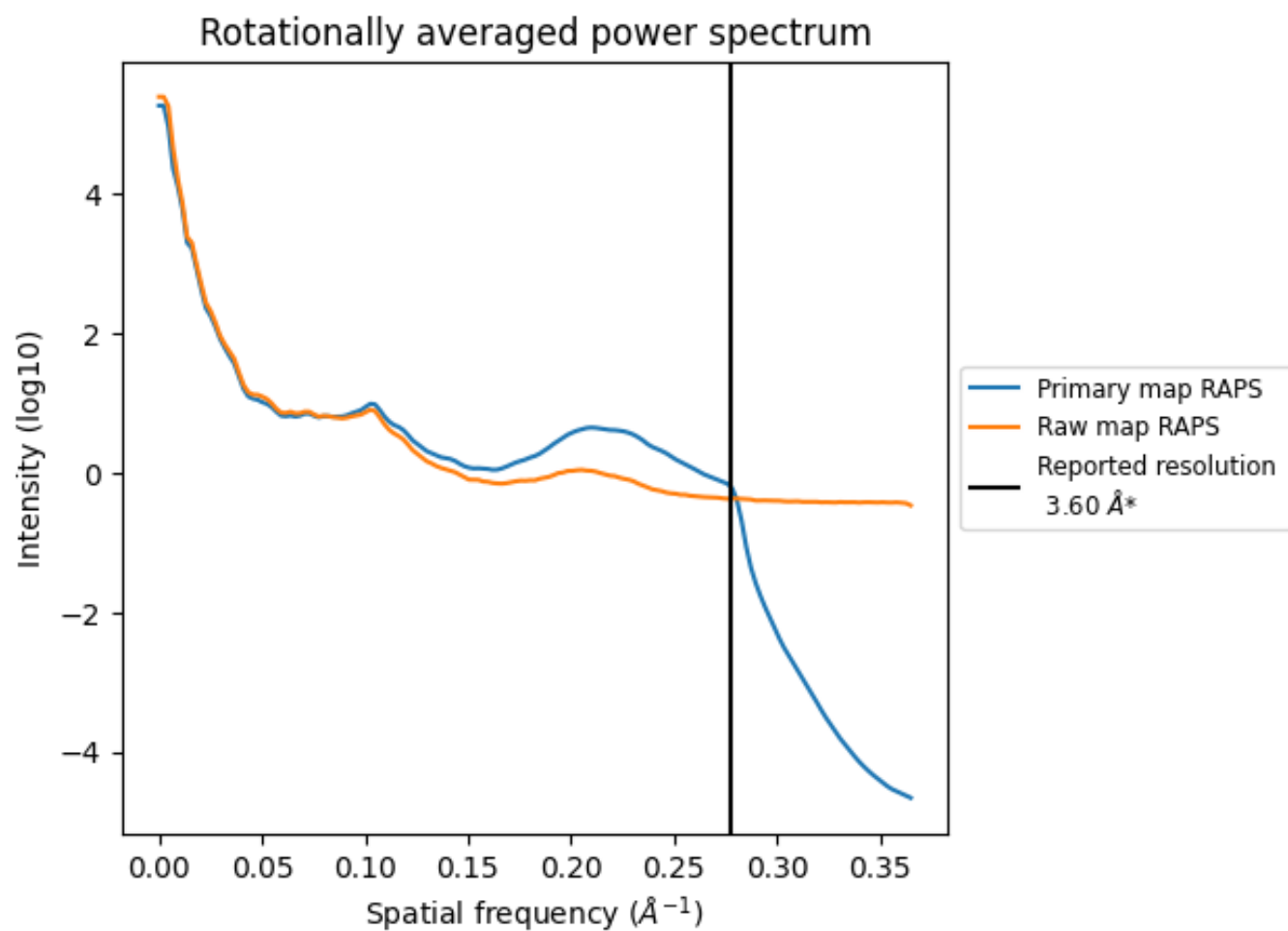
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 224 nm³; this corresponds to an approximate mass of 203 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 ⓘ

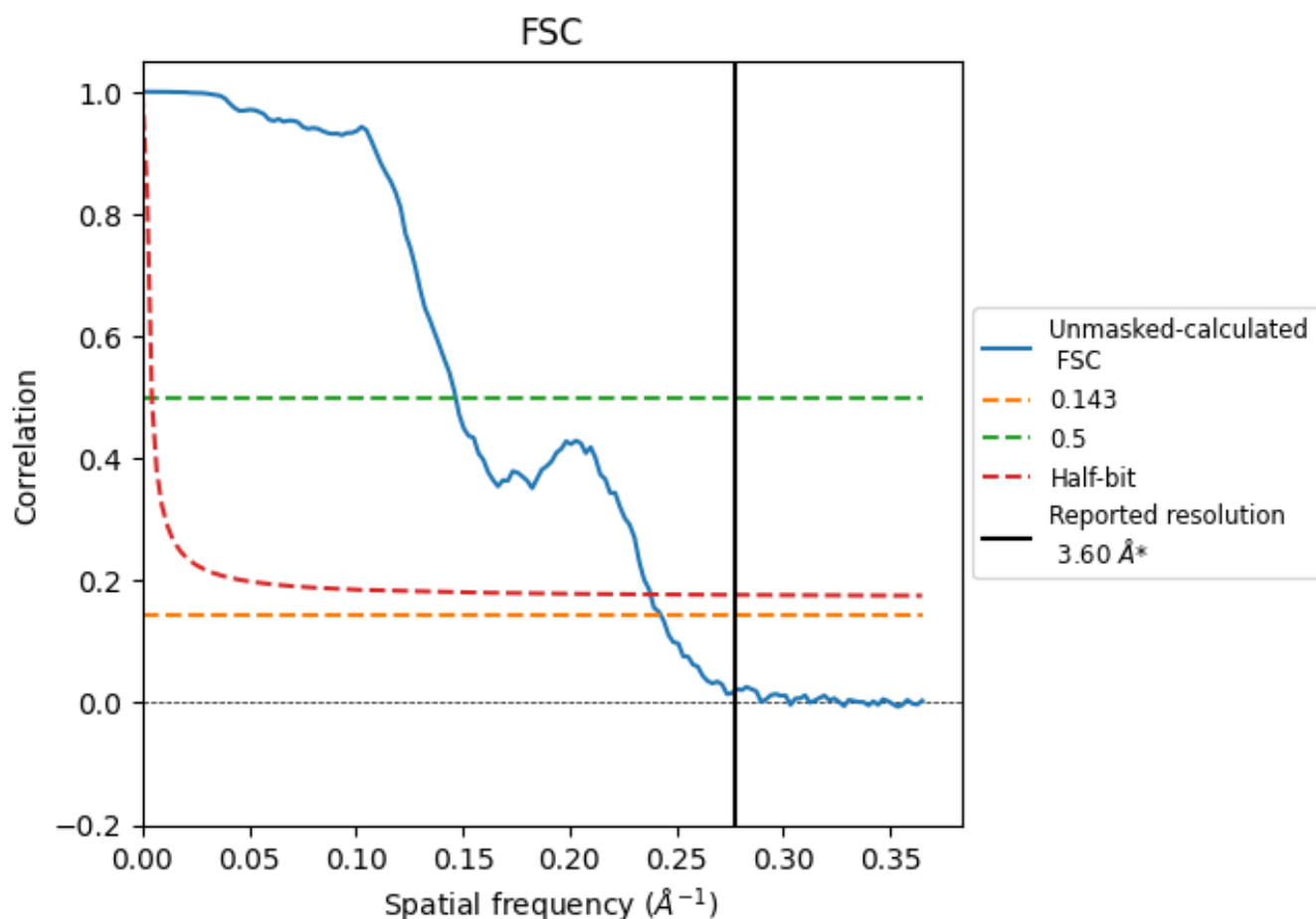


*Reported resolution corresponds to spatial frequency of 0.278 $\text{\AA}^{-1}$

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 0.278 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

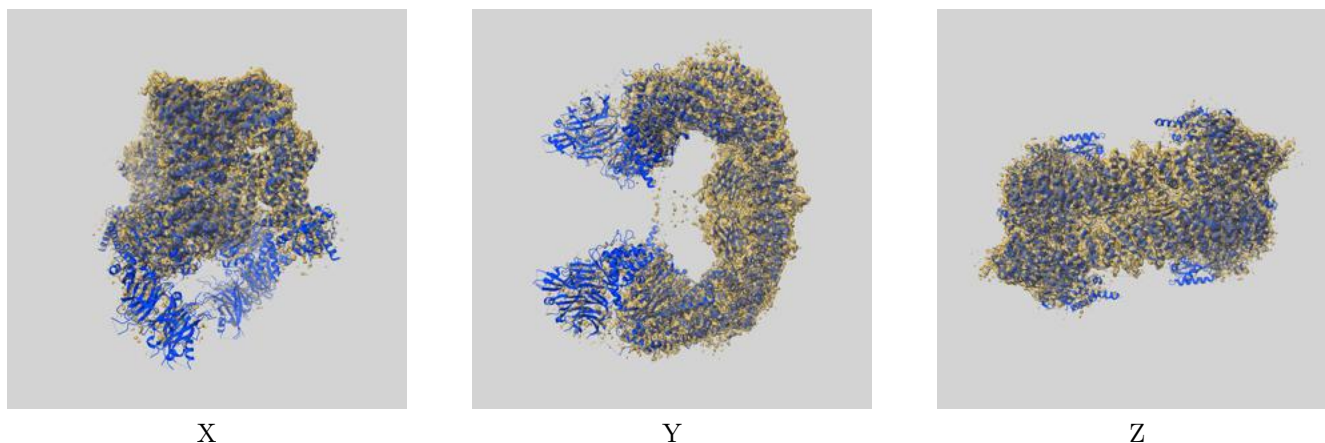
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.12	6.82	4.20

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

9 Map-model fit [i](#)

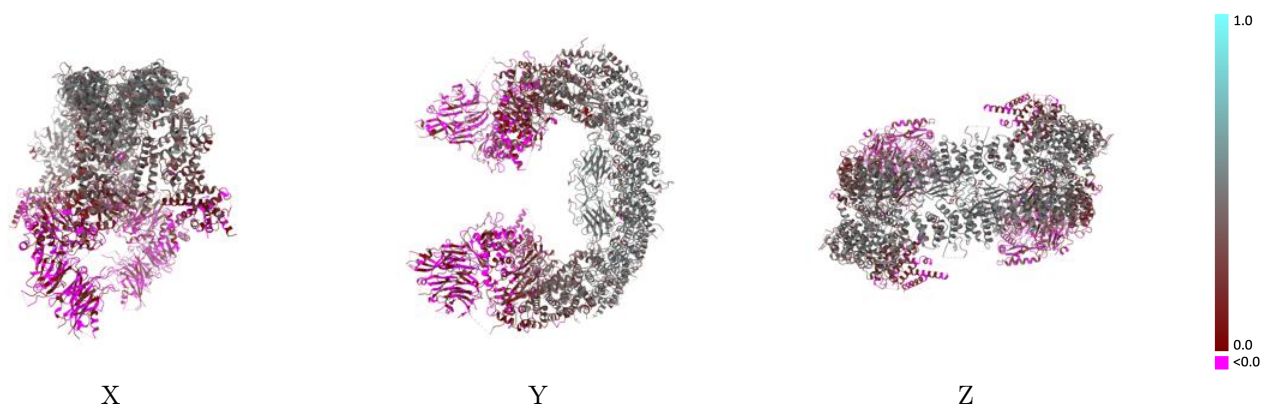
This section contains information regarding the fit between EMDB map EMD-35759 and PDB model 8IVQ. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



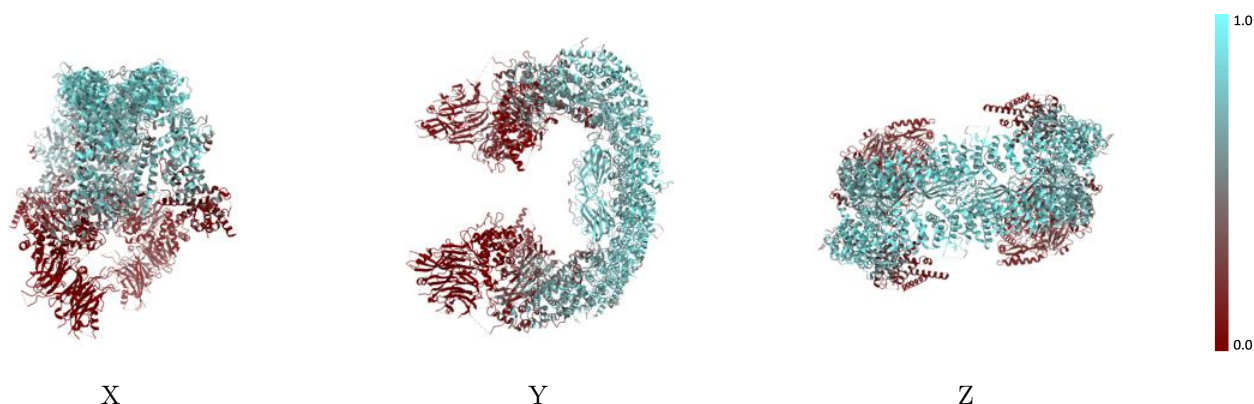
The images above show the 3D surface view of the map at the recommended contour level 0.03 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



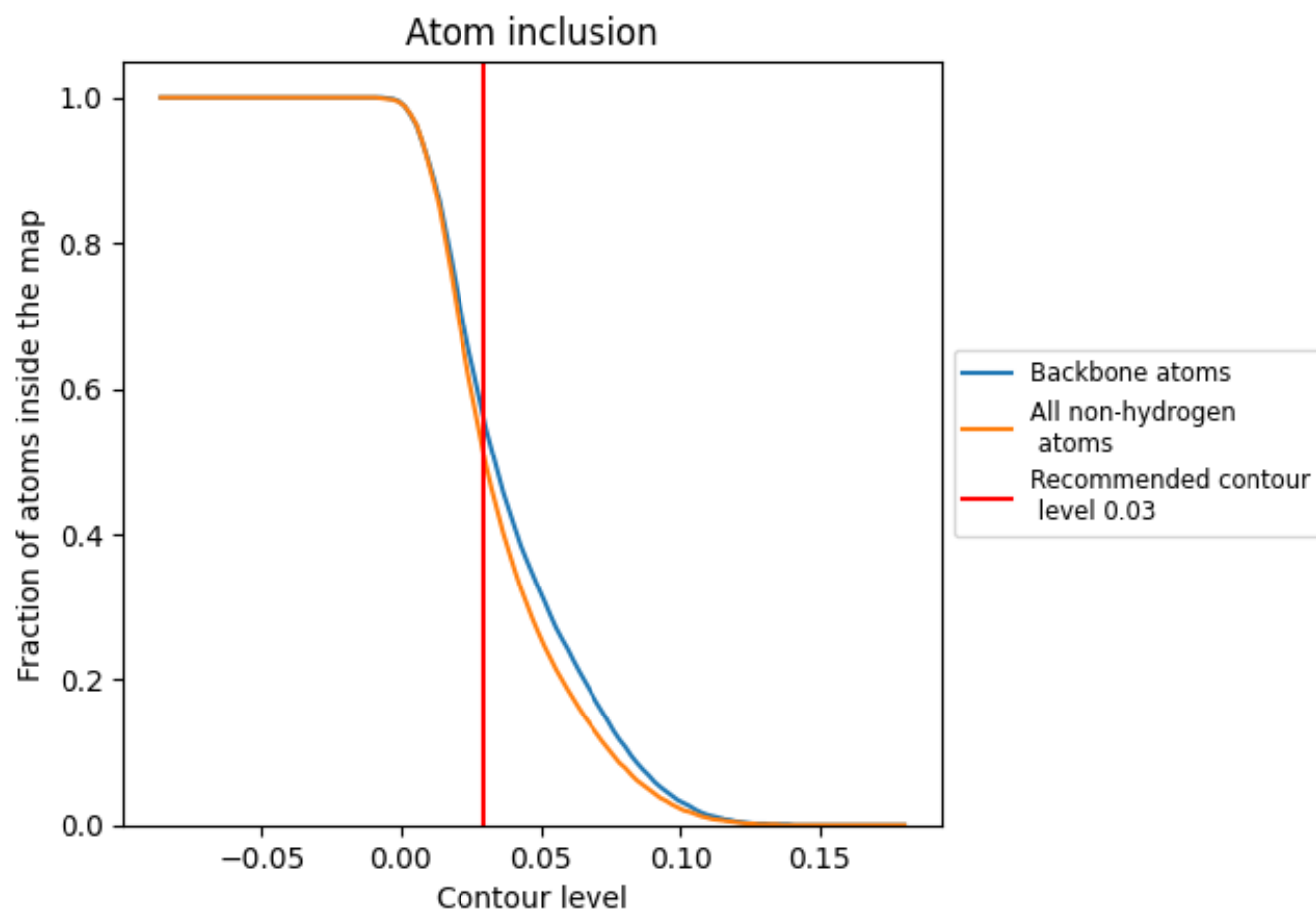
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.03).

9.4 Atom inclusion [i](#)



At the recommended contour level, 55% of all backbone atoms, 50% 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 (0.03) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5050	0.2990
A	0.5050	0.2990
B	0.5050	0.2990

