



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:45 PM UTC

PDB ID : 8GHG / pdb_00008ghg
EMDB ID : EMD-40045
Title : Cryo-EM structure of hSlo1 in digitonin, Ca²⁺-free and EDTA-free
Authors : Tao, X.; Zhao, C.; MacKinnon, R.
Deposited on : 2023-03-10
Resolution : 3.30 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

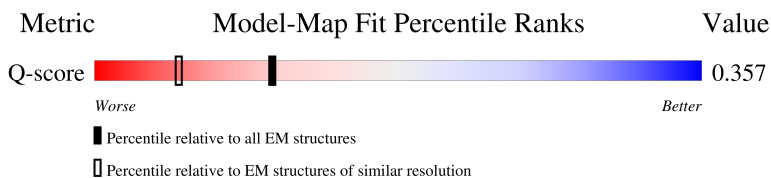
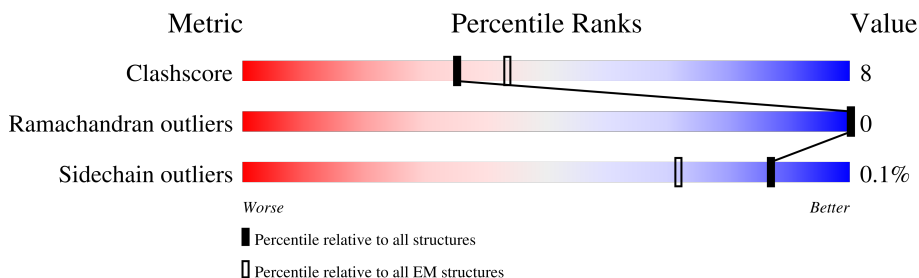
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.30 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	15087 (2.80 - 3.80)

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	1072	10% 58% 18% 24%
1	B	1072	10% 61% 15% 24%
1	C	1072	12% 64% 15% 20%
1	D	1072	12% 64% 15% 21%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 26659 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 Calcium-activated potassium channel subunit alpha-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	816	Total	C	N	O	S	1	0
			6533	4241	1060	1189	43		
1	C	853	Total	C	N	O	S	1	0
			6802	4414	1109	1236	43		
1	B	817	Total	C	N	O	S	1	0
			6549	4254	1062	1190	43		
1	D	849	Total	C	N	O	S	1	0
			6775	4398	1105	1229	43		

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP Q12791
A	-14	ALA	-	expression tag	UNP Q12791
A	-13	PRO	-	expression tag	UNP Q12791
A	-12	SER	-	expression tag	UNP Q12791
A	-11	ARG	-	expression tag	UNP Q12791
A	-10	LEU	-	expression tag	UNP Q12791
A	-9	GLU	-	expression tag	UNP Q12791
A	-8	GLU	-	expression tag	UNP Q12791
A	-7	GLU	-	expression tag	UNP Q12791
A	-6	LEU	-	expression tag	UNP Q12791
A	-5	ARG	-	expression tag	UNP Q12791
A	-4	ARG	-	expression tag	UNP Q12791
A	-3	ARG	-	expression tag	UNP Q12791
A	-2	LEU	-	expression tag	UNP Q12791
A	-1	THR	-	expression tag	UNP Q12791
A	0	GLU	-	expression tag	UNP Q12791
A	1	PRO	-	expression tag	UNP Q12791
C	-15	MET	-	expression tag	UNP Q12791
C	-14	ALA	-	expression tag	UNP Q12791
C	-13	PRO	-	expression tag	UNP Q12791
C	-12	SER	-	expression tag	UNP Q12791
C	-11	ARG	-	expression tag	UNP Q12791

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	LEU	-	expression tag	UNP Q12791
C	-9	GLU	-	expression tag	UNP Q12791
C	-8	GLU	-	expression tag	UNP Q12791
C	-7	GLU	-	expression tag	UNP Q12791
C	-6	LEU	-	expression tag	UNP Q12791
C	-5	ARG	-	expression tag	UNP Q12791
C	-4	ARG	-	expression tag	UNP Q12791
C	-3	ARG	-	expression tag	UNP Q12791
C	-2	LEU	-	expression tag	UNP Q12791
C	-1	THR	-	expression tag	UNP Q12791
C	0	GLU	-	expression tag	UNP Q12791
C	1	PRO	-	expression tag	UNP Q12791
B	-15	MET	-	expression tag	UNP Q12791
B	-14	ALA	-	expression tag	UNP Q12791
B	-13	PRO	-	expression tag	UNP Q12791
B	-12	SER	-	expression tag	UNP Q12791
B	-11	ARG	-	expression tag	UNP Q12791
B	-10	LEU	-	expression tag	UNP Q12791
B	-9	GLU	-	expression tag	UNP Q12791
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B	-6	LEU	-	expression tag	UNP Q12791
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B	-4	ARG	-	expression tag	UNP Q12791
B	-3	ARG	-	expression tag	UNP Q12791
B	-2	LEU	-	expression tag	UNP Q12791
B	-1	THR	-	expression tag	UNP Q12791
B	0	GLU	-	expression tag	UNP Q12791
B	1	PRO	-	expression tag	UNP Q12791
D	-15	MET	-	expression tag	UNP Q12791
D	-14	ALA	-	expression tag	UNP Q12791
D	-13	PRO	-	expression tag	UNP Q12791
D	-12	SER	-	expression tag	UNP Q12791
D	-11	ARG	-	expression tag	UNP Q12791
D	-10	LEU	-	expression tag	UNP Q12791
D	-9	GLU	-	expression tag	UNP Q12791
D	-8	GLU	-	expression tag	UNP Q12791
D	-7	GLU	-	expression tag	UNP Q12791
D	-6	LEU	-	expression tag	UNP Q12791
D	-5	ARG	-	expression tag	UNP Q12791
D	-4	ARG	-	expression tag	UNP Q12791
D	-3	ARG	-	expression tag	UNP Q12791

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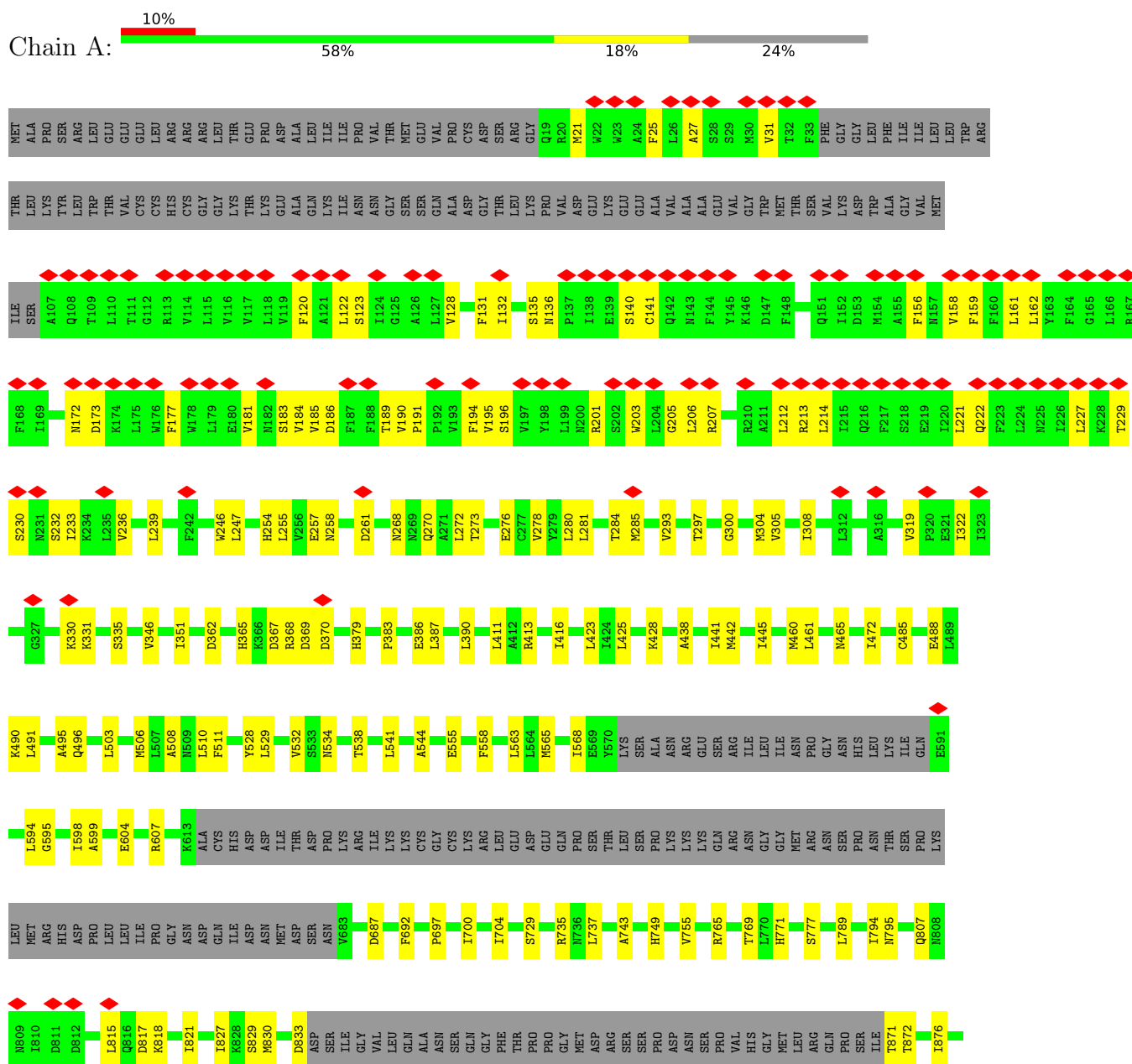
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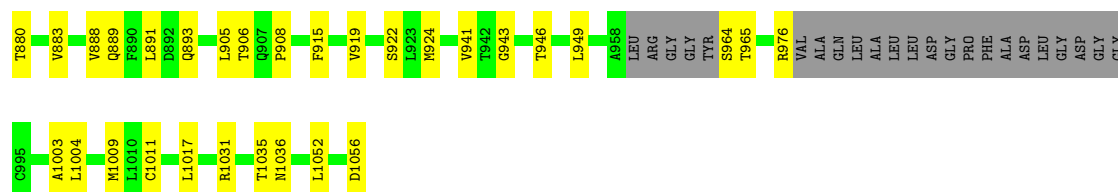
Chain	Residue	Modelled	Actual	Comment	Reference
D	-2	LEU	-	expression tag	UNP Q12791
D	-1	THR	-	expression tag	UNP Q12791
D	0	GLU	-	expression tag	UNP Q12791
D	1	PRO	-	expression tag	UNP Q12791

3 Residue-property plots

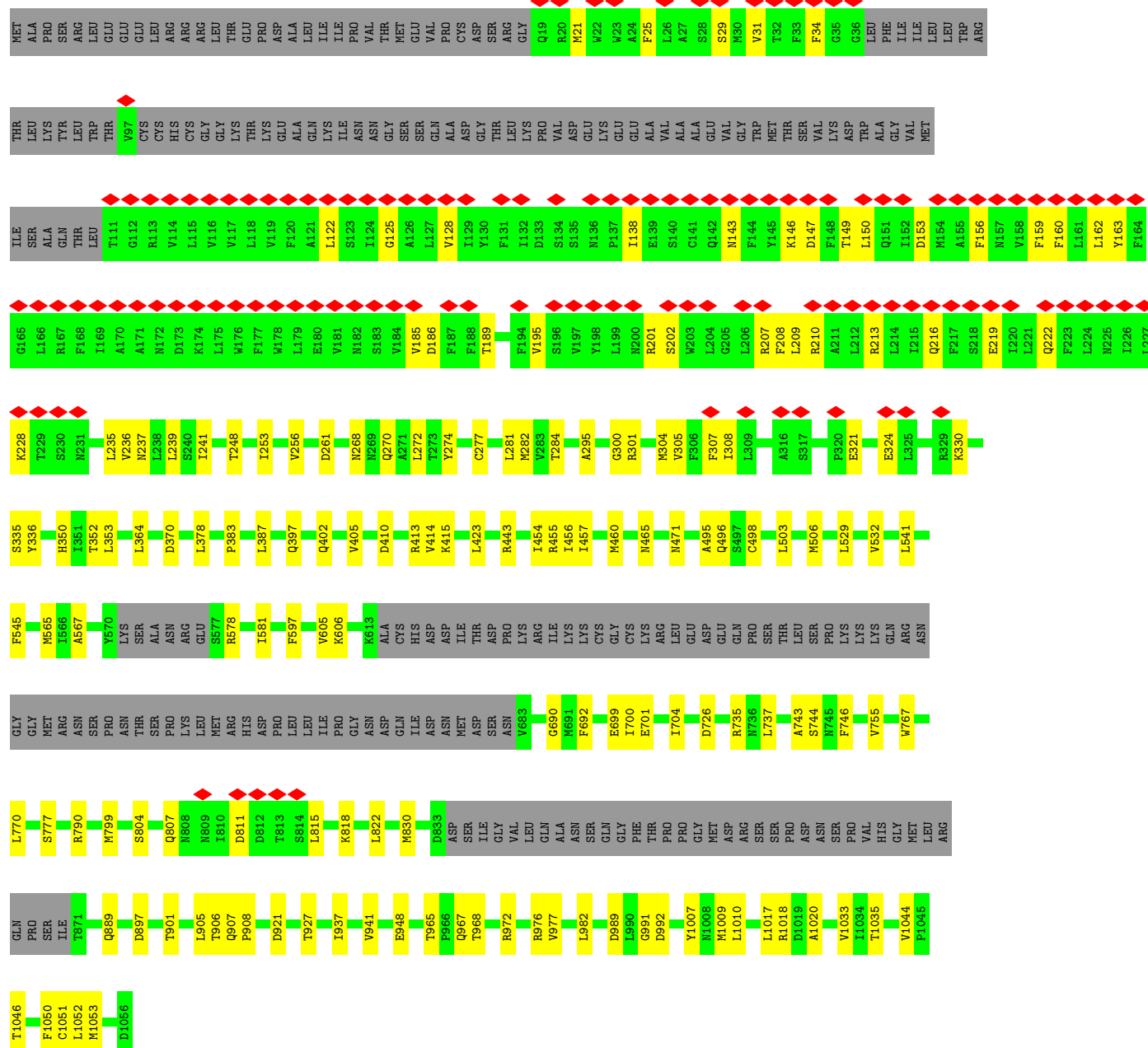
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Calcium-activated potassium channel subunit alpha-1





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W1008	W1009	L1010	I1014	R1018	S1026	Q1027	C1028	V1033	I1034	T1035	V1044	P1045	T1046	F1050	M1053	D1056	ASN	SER	PRO	VAL	HIS	GLY	MET	LEU	ARG	GLN	PRO	SER	ILE	T871	V888	D897	E902	L903	Y904	L905	T906	D921	T927	N930	D931	N932	I933	L934	I937	L940	V941	E950	I953	E956	R960	R972	R976	V977	D989	D992	A1003	Y1007	ASP	ARG	GLY	VAL	ILE	SER	ASN	GLN	ALA	LEU	THR	PRO	GLY	MET	ASP	ARG	L737	N736	R735	S729	THR	SER	PRO	D726	C722	R707	I704	V703	K702	E701	I700	E699	K698	F692	V683	ASN	SER	ASP	MET	ILE	ASP	ASN	GLY	PRO	C612	K613	ALA	CYS	HIS	ILE	ASP	ASP	ASP	ASP	THR	ILE	ASP	M460	I457	I456	R455	I454	N449	K448	D261	V256	N255	V181	E180	L179	W178	F177	W176	L175	K174	D173	N172	A171	A170	I169	F168	R167	Y130	I129	V128	L127	A126	G125	I124	S123	L122	A121	F120	V119	L118	V117	V116	L115	V114	R113	G112	T111	L110	T109	GLN	ALA	SER	Y166	G165	F164	Y163	L161	F160	F159	V158	N157	F156	A155	M154	D153	I152	Q151	L150	T149	F148	D147	K146	Y145	F144	N143	Q142	C141	S140	E139	I138	P137	N136	S135	S134	D133	V195	S196	V197	Y198	L199	G300	N200	R201	S202	W203	L204	G205	L206	R207	F208	L209	R210	A211	L212	R213	L214	I215	Q216	F217	S218	E219	I220	L221	Q222	F223	L224	N225	I226	L227	K228	T229	I326	E324	I323	I322	E321	P320	V319	Y318	S317	A316	L312	G311	G310	L309	I308	F307	V306	F305	M304	F303	L302	R301	L299	T298	T297	T287	W282	L272	F266	D261	V256	N255	V181	E180	L179	W178	F177	W176	L175	K174	D173	N172	A171	A170	I169	F168	R167	Y130	I129	V128	L127	A126	G125	I124	S123	L122	A121	F120	V119	L118	V117	V116	L115	V114	R113	G112	T111	L110	T109	GLN	ALA	SER	Y166	G165	F164	Y163	L161	F160	F159	V158	N157	F156	A155	M154	D153	I152	Q151	L150	T149	F148	D147	K146	Y145	F144	N143	Q142	C141	S140	E139	I138	P137	N136	S135	S134	D133	V195	S196	V197	Y198	L199	G300	N200	R201	S202	W203	L204	G205	L206	R207	F208	L209	R210	A211	L212	R213	L214	I215	Q216	F217	S218	E219	I220	L221	Q222	F223	L224	N225	I226	L227	K228	T229	I326	E324	I323	I322	E321	P320	V319	Y318	S317	A316	L312	G311	G310	L309	I308	F307	V306	F305	M304	F303	L302	R301	L299	T298	T297	T287	W282	L272	F266	D261	V256	N255	V181	E180	L179	W178	F177	W176	L175	K174	D173	N172	A171	A170	I169	F168	R167	Y130	I129	V128	L127	A126	G125	I124	S123	L122	A121	F120	V119	L118	V117	V116	L115	V114	R113	G112	T111	L110	T109	GLN	ALA	SER	Y166	G165	F164	Y163	L161	F160	F159	V158	N157	F156	A155	M154	D153	I152	Q151	L150	T149	F148	D147	K146	Y145	F144	N143	Q142	C141	S140	E139	I138	P137	N136	S135	S134	D133	V195	S196	V197	Y198	L199	G300	N200	R201	S202	W203	L204	G205	L206	R207	F208	L209	R210	A211	L212	R213	L214	I215	Q216	F217	S218	E219	I220	L221	Q222	F223	L224	N225	I226	L227	K228	T229	I326	E324	I323	I322	E321	P320	V319	Y318	S317	A316	L312	G311	G310	L309	I308	F307	V306	F305	M304	F303	L302	R301	L299	T298	T297	T287	W282	L272	F266	D261	V256	N255	V181	E180	L179	W178	F177	W176	L175	K174	D173	N172	A171	A170	I169	F168	R167	Y130	I129	V128	L127	A126	G125	I124	S123	L122	A121	F120	V119	L118	V117	V116	L115	V114	R113	G112	T111	L110	T109	GLN	ALA	SER	Y166	G165	F164	Y163	L161	F160	F159	V158	N157	F156	A155	M154	D153	I152	Q151	L150	T149	F148	D147	K146	Y145	F144	N143	Q142	C141	S140	E139	I138	P137	N136	S135	S134	D133	V195	S196	V197	Y198	L199	G300	N200	R201	S202	W203	L204	G205	L206	R207	F208	L209	R210	A211	L212	R213	L214	I215	Q216	F217	S218	E219	I220	L221	Q222	F223	L224	N225	I226	L227	K228	T229	I326	E324	I323	I322	E321	P320	V319	Y318	S317	A316	L312	G311	G310	L309	I308	F307	V306	F305	M304	F303	L302	R301	L299	T298	T297	T287	W282	L272	F266	D261	V256	N255	V181	E180	L179	W178	F177	W176	L175	K174	D173	N172	A171	A170	I169	F168	R167	Y130	I129	V128	L127	A126	G125	I124	S123	L122	A121	F120	V119	L118	V117	V116	L115	V114	R113	G112	T111	L110	T109	GLN	ALA	SER	Y166	G165	F164	Y163	L161	F160	F159	V158	N157	F156	A155	M154	D153	I152	Q151	L150	T149	F148	D147	K146	Y145	F144	N143	Q142	C141	S140	E139	I138	P137	N136	S135	S134	D133	V195	S196	V197	Y198	L199	G300	N200	R201	S202	W203	L204	G205	L206	R207	F208	L209	R210	A211	L212	R213	L214	I215	Q216	F217	S218	E219	I220	L221	Q222	F223	L224	N225	I226	L227	K228	T229	I326	E324	I323	I322	E321	P320	V319	Y318	S317	A316	L312	G311	G310	L309	I308	F307	V306	F305	M304	F303	L302	R301	L299	T298	T297	T287	W282	L272	F266	D261	V256	N255	V181	E180	L179	W178	F177	W176	L175	K174	D173	N172	A171	A170	I169	F168	R167	Y130	I129	V128	L127	A126	G125	I124	S123	L122	A121	F120	V119	L118	V117	V116	L115	V114	R113	G112	T111	L110	T109	GLN	ALA	SER	Y166	G165	F164	Y163	L161	F160	F159	V158	N157	F156	A155	M154	D153	I152	Q151	L150	T149	F148	D147	K146	Y145	F144	N143	Q142	C141	S140	E139	I138	P137	N136	S135	S134	D133	V195	S196	V197	Y198	L199	G300	N200	R201	S202	W203	L204	G205	L206	R207	F208	L209	R210	A211	L212	R213	L214	I215	Q216	F217	S218	E219	I220	L221	Q222	F223	L224	N225	I226	L227	K228	T229	I326	E324	I323	I322	E321	P320	V319	Y318	S317	A316	L312	G311	G310	L309	I308	F307	V306	F305	M304	F303	L302	R301	L299	T298	T297	T287	W282	L272	F266	D261	V256	N255	V181	E180	L179	W178	F177	W176	L175	K174	D173	N172	A171	A170	I169	F168	R167	Y130	I129	V128	L127	A126	G125	I124	S123	L122	A121	F120	V119	L118	V117	V116	L115	V114	R113	G112	T111	L110	T109	GLN	ALA	SER	Y166	G165	F164	Y163	L161	F160	F159	V158	N157	F156	A155	M154	D153	I152	Q151	L150	T149	F148	D147	K146	Y145	F144	N143	Q142	C141	S140	E139	I138	P137	N136	S135	S134	D133	V195	S196	V197	Y198	L199	G300	N200	R201	S202	W203	L204	G205	L206	R207	F208	L209	R210	A211	L212	R213	L214	I215	Q216	F217	S218	E219	I220	L221	Q222	F223	L224	N225	I226	L227	K228	T229	I326	E324	I323	I322	E321	P320	V319	Y318	S317	A316	L312	G311	G310	L309	I308	F307	V306	F305	M304	F303	L302	R301	L299	T298	T297	T287	W282	L272	F266	D261	V256	N255	V181	E180	L179	W178	F177	W176	L175	K174	D173	N172	A171	A170	I169	F168	R167	Y130	I129	V128	L127	A126	G125	I124	S123	L122	A121	F120	V119	L118	V117	V116	L115	V114	R113	G112	T111	L110	T109	GLN	ALA	SER	Y166	G165	F164	Y163	L161	F160	F159	V158	N157	F156	A155	M154	D153	I152	Q151	L150	T149	F148	D147	K146	Y145	F144	N143	Q142	C141	S140	E139	I138	P137	N136	S135	S134	D133	V195	S196	V197	Y198	L199	G300	N200	R201	S202	W203	L204	G205	L206	R207	F208	L209	R210	A211	L212	R213	L214	I215	Q216	F217	S218	E219	I220	L221	Q222	F223	L224	N225	I226	L227	K228	T229	I326	E324	I323	I322	E321	P320	V319	Y318	S317	A316	L312	G311	G310	L309	I308	F307	V306	F305	M304	F303	L302	R301	L299	T298	T297	T287	W282	L272	F266	D261	V256	N255	V181	E180	L179	W178	F177	W176	L175	K174	D173	N172	A171	A170	I169	F168	R167	Y130	I129	V128	L127	A126	G125	I124	S123	L122	A121	F120	V119	L118	V117	V116	L115	V114	R113	G112	T111	L110	T109	GLN	ALA	SER	Y166	G165	F164	Y163	L161	F160	F159	V158	N157	F156	A155	M154	D153	I152	Q151	L150	T149	F148	D147	K146	Y145	F144	N143	Q142	C141	S140	E139	I138	P137	N136	S135	S134	D133	V195	S196	V197	Y198	L199	G300	N200	R201	S202	W203	L204	G205	L206	R207	F208	L209	R210	A211	L212	R213	L214	I215	Q216	F217	S218	E219	I220	L221	Q222	F223	L224	N225	I226	L227	K228	T229	I326	E324	I323	I322	E321	P320	V319	Y318	S317	A316	L312	G311	G310	L309	I308	F307	V306	F305	M304	F303	L302	R301	L299	T298	T297	T287	W282	L272	F266	D261	V256	N255	V181	E180	L179	W178	F177	W176	L175	K174	D173	N172	A171	A170	I169	F168	R167	Y130	I129	V128	L127	A126	G125	I124	S123	L122	A121	F120	V119	L118	V117	V116	L115	V114	R113	G112	T111	L110	T109	GLN	ALA	SER	Y166	G165	F164	Y163	L161	F160	F159	V158	N157	F156	A155	M154	D153	I152	Q151	L150	T149	F148	D147	K146	Y145	F144	N143	Q142	C141	S140	E139	I138	P137	N136	S135	S134	D133	V195	S196	V197	Y198	L199	G300	N200	R201	S202	W203	L204	G205	L206	R207	F208	L209	R210	A211	L212	R213	L214	I215	Q216	F217	S218	E219	I220	L221	Q222	F223	L224	N225	I226	L227	K228	T229	I326	E324	I323	I322	E321	P320	V319	Y318	S317	A316	L312	G311	G310	L309	I308	F307	V306	F305	M304	F303	L302	R301	L299	T298
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4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	123286	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 ($e^-/\text{\AA}^2$)	51.4	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.967	Depositor
Minimum map value	-0.314	Depositor
Average map value	0.016	Depositor
Map value standard deviation	0.061	Depositor
Recommended contour level	0.28	Depositor
Map size (Å)	276.48, 276.48, 276.48	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.08, 1.08, 1.08	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	0.13	0/6681	0.37	0/9062
1	B	0.14	0/6698	0.39	2/9085 (0.0%)
1	C	0.13	0/6957	0.37	0/9436
1	D	0.12	0/6929	0.34	0/9399
All	All	0.13	0/27265	0.37	2/36982 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	30	MET	CB-CG-SD	5.15	128.15	112.70
1	B	282	MET	CG-SD-CE	5.10	112.12	100.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6533	0	6499	120	0
1	B	6549	0	6512	103	0
1	C	6802	0	6771	104	0
1	D	6775	0	6757	105	0
All	All	26659	0	26539	420	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 8.

All (420) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:794:ILE:HG21	1:A:827:ILE:HD11	1.64	0.80
1:A:491:LEU:HD12	1:A:737:LEU:HB2	1.67	0.75
1:A:445:ILE:HD13	1:A:472:ILE:HD12	1.69	0.75
1:B:246:TRP:HZ2	1:B:278:VAL:HG13	1.51	0.74
1:B:287:THR:HB	1:D:287:THR:HB	1.71	0.72
1:D:482:ASP:HB3	1:D:934:LEU:HD13	1.70	0.71
1:A:21:MET:HE1	1:A:201:ARG:HD3	1.74	0.70
1:C:455:ARG:NH2	1:C:927:THR:O	2.26	0.68
1:B:211:ALA:HA	1:B:214:LEU:HD23	1.76	0.67
1:B:755:VAL:HG12	1:B:777:SER:HB2	1.77	0.67
1:A:284:THR:HG21	1:A:304:MET:HE1	1.77	0.67
1:B:794:ILE:HG21	1:B:827:ILE:HD11	1.77	0.66
1:A:506:MET:HE1	1:A:1035:THR:HA	1.78	0.65
1:A:906:THR:HG22	1:A:908:PRO:HD2	1.78	0.65
1:B:800:CYS:HB3	1:B:878:ILE:HG22	1.79	0.65
1:A:346:VAL:HG21	1:A:416:ILE:HG22	1.79	0.65
1:C:29:SER:HA	1:C:195:VAL:HG21	1.77	0.65
1:B:555:GLU:HG3	1:B:1004:LEU:HB3	1.81	0.63
1:C:503:LEU:HD22	1:C:977:VAL:HG11	1.81	0.63
1:A:558:PHE:HE1	1:A:565:MET:H	1.46	0.63
1:A:1017:LEU:HA	1:A:1031:ARG:HA	1.81	0.63
1:A:132:ILE:O	1:A:136:ASN:ND2	2.31	0.62
1:A:335:SER:HA	1:A:413:ARG:HG3	1.81	0.62
1:A:815:LEU:HD12	1:A:818:LYS:HD3	1.81	0.62
1:D:454:ILE:HG23	1:D:456:ILE:HD11	1.80	0.62
1:B:727:VAL:O	1:B:765:ARG:NH1	2.33	0.62
1:D:238:LEU:HD21	1:D:322:ILE:HB	1.82	0.61
1:D:1003:ALA:HB1	1:D:1009:MET:HB2	1.82	0.61
1:B:491:LEU:HD12	1:B:737:LEU:HB2	1.83	0.61
1:A:305:VAL:HG23	1:C:282:MET:HG3	1.83	0.61
1:A:555:GLU:HA	1:A:558:PHE:HB3	1.81	0.61
1:D:744:SER:HB3	1:D:972:ARG:HD2	1.81	0.61
1:D:536:MET:HE1	1:D:933:ILE:HD12	1.83	0.60
1:C:305:VAL:HG23	1:B:282:MET:HG3	1.82	0.60
1:C:906:THR:HG22	1:C:908:PRO:HD2	1.82	0.60
1:C:378:LEU:HD11	1:C:414:VAL:HG21	1.83	0.60
1:C:471:ASN:OD1	1:B:786:ARG:NH2	2.35	0.60
1:A:541:LEU:HD21	1:A:544:ALA:HB3	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:TRP:CZ2	1:B:278:VAL:HG13	2.35	0.60
1:B:411:LEU:HD12	1:B:416:ILE:HD13	1.82	0.60
1:C:147:ASP:HB3	1:C:150:LEU:HD23	1.84	0.60
1:A:893:GLN:HE22	1:D:473:PRO:HB2	1.67	0.59
1:A:254:HIS:O	1:A:258:ASN:ND2	2.35	0.59
1:A:383:PRO:HB3	1:A:387:LEU:HD23	1.84	0.59
1:A:976:ARG:HB3	1:A:1052:LEU:HD23	1.84	0.59
1:D:254:HIS:NE2	1:D:272:LEU:O	2.35	0.59
1:A:203:TRP:O	1:A:207:ARG:NH1	2.35	0.59
1:C:138:ILE:HD12	1:C:201:ARG:HH12	1.66	0.59
1:A:755:VAL:HG12	1:A:777:SER:HB2	1.83	0.59
1:D:1007:TYR:HB2	1:D:1009:MET:HG2	1.83	0.59
1:A:280:LEU:HD21	1:A:293:VAL:HG23	1.85	0.59
1:C:1017:LEU:HB2	1:C:1020:ALA:HB2	1.85	0.59
1:B:1016:ARG:NH2	1:B:1042:GLU:O	2.35	0.59
1:B:975:CYS:O	1:B:1052:LEU:N	2.34	0.58
1:D:297:THR:HG23	1:D:300:GLY:H	1.68	0.58
1:B:997:GLY:HA2	1:B:1000:PHE:CE1	2.38	0.58
1:D:930:ASN:HB3	1:D:933:ILE:HG12	1.84	0.58
1:C:597:PHE:HD2	1:C:605:VAL:HG13	1.69	0.58
1:D:118:LEU:HD23	1:D:216:GLN:HG2	1.86	0.58
1:D:1014:ILE:HB	1:D:1034:ILE:HB	1.86	0.58
1:B:117:VAL:HA	1:B:120:PHE:CE1	2.39	0.57
1:C:815:LEU:HB3	1:C:818:LYS:HD3	1.87	0.57
1:A:365:HIS:ND1	1:A:367:ASP:OD1	2.38	0.57
1:A:871:THR:OG1	1:A:872:THR:N	2.37	0.57
1:D:888:VAL:HG11	1:D:906:THR:HG21	1.86	0.57
1:B:449:ASN:ND2	1:D:897:ASP:OD2	2.32	0.57
1:A:261:ASP:OD2	1:A:268:ASN:ND2	2.39	0.56
1:D:956:GLU:OE2	1:D:960:ARG:NH1	2.38	0.56
1:D:976:ARG:NE	1:D:1053:MET:SD	2.75	0.56
1:C:304:MET:HA	1:C:307:PHE:HD2	1.70	0.56
1:A:411:LEU:HD12	1:A:416:ILE:HD13	1.88	0.56
1:B:273:THR:OG1	1:B:276:GLU:OE1	2.23	0.56
1:D:566:ILE:HG22	1:D:1010:LEU:HD21	1.88	0.56
1:D:729:SER:O	1:D:765:ARG:NH2	2.39	0.56
1:A:177:PHE:O	1:A:183:SER:OG	2.17	0.56
1:C:222:GLN:HE22	1:C:228:LYS:HA	1.70	0.55
1:D:430:CYS:O	1:D:808:ASN:ND2	2.39	0.55
1:A:281:LEU:HB2	1:A:285:MET:HE1	1.87	0.55
1:A:496:GLN:HB3	1:A:503:LEU:HD23	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:353:LEU:HD22	1:B:386:GLU:HG3	1.87	0.55
1:B:548:LEU:HB2	1:B:553:VAL:HG11	1.88	0.55
1:A:538:THR:HB	1:A:594:LEU:HD11	1.89	0.55
1:C:1007:TYR:HB2	1:C:1009:MET:HB2	1.88	0.55
1:B:142:GLN:NE2	1:B:143:ASN:O	2.40	0.55
1:C:304:MET:O	1:C:308:ILE:HG12	2.07	0.55
1:D:496:GLN:HB3	1:D:503:LEU:HD23	1.89	0.55
1:B:346:VAL:HG21	1:B:416:ILE:HG22	1.88	0.55
1:D:120:PHE:HB2	1:D:216:GLN:HE22	1.72	0.55
1:C:496:GLN:HB3	1:C:503:LEU:HD23	1.89	0.54
1:A:222:GLN:HE21	1:A:233:ILE:HG21	1.72	0.54
1:B:1017:LEU:HB2	1:B:1020:ALA:HB2	1.89	0.54
1:A:273:THR:N	1:A:276:GLU:OE2	2.32	0.54
1:D:755:VAL:HG12	1:D:777:SER:HB2	1.90	0.54
1:A:510:LEU:HD22	1:A:598:ILE:HD11	1.90	0.54
1:B:430:CYS:SG	1:B:431:ALA:N	2.80	0.54
1:A:25:PHE:HA	1:A:195:VAL:HG21	1.89	0.54
1:A:729:SER:O	1:A:765:ARG:NH2	2.40	0.54
1:C:1044:VAL:HG12	1:C:1046:THR:H	1.71	0.53
1:D:506:MET:SD	1:D:1035:THR:OG1	2.61	0.53
1:D:261:ASP:OD1	1:D:297:THR:OG1	2.26	0.53
1:D:253:ILE:HA	1:D:256:VAL:HG12	1.90	0.53
1:D:529:LEU:HA	1:D:532:VAL:HG12	1.89	0.53
1:A:976:ARG:HA	1:A:1011:CYS:HA	1.90	0.53
1:C:495:ALA:HB2	1:C:737:LEU:HD12	1.91	0.53
1:A:735:ARG:NH1	1:A:769:THR:OG1	2.42	0.52
1:B:430:CYS:O	1:B:808:ASN:ND2	2.43	0.52
1:B:790:ARG:NH2	1:B:831:GLN:O	2.36	0.52
1:A:1017:LEU:HB3	1:A:1031:ARG:HG2	1.91	0.52
1:C:976:ARG:NE	1:C:1053:MET:SD	2.78	0.52
1:A:230:SER:HA	1:A:233:ILE:HG12	1.92	0.52
1:C:222:GLN:O	1:C:228:LYS:NZ	2.43	0.52
1:C:529:LEU:HA	1:C:532:VAL:HG12	1.91	0.52
1:C:31:VAL:HA	1:C:34:PHE:HD2	1.75	0.52
1:C:270:GLN:HB3	1:C:272:LEU:HD23	1.90	0.52
1:B:282:MET:O	1:B:286:SER:OG	2.26	0.52
1:D:746:PHE:HD1	1:D:976:ARG:HH11	1.57	0.52
1:A:330:LYS:NZ	1:A:331:LYS:O	2.39	0.52
1:C:186:ASP:HA	1:C:189:THR:HG22	1.92	0.52
1:B:709:GLU:HA	1:B:712:MET:HG3	1.92	0.52
1:D:503:LEU:HD22	1:D:977:VAL:HG11	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:274:TYR:HA	1:C:277:CYS:SG	2.50	0.51
1:D:322:ILE:O	1:D:326:ILE:HG12	2.10	0.51
1:D:460:MET:N	1:D:484:ILE:O	2.38	0.51
1:C:565:MET:HE1	1:C:597:PHE:CE1	2.45	0.51
1:C:402:GLN:O	1:C:413:ARG:NH2	2.42	0.51
1:A:123:SER:OG	1:A:213:ARG:NH2	2.44	0.51
1:A:272:LEU:HD12	1:A:276:GLU:HG3	1.93	0.51
1:B:795:ASN:HA	1:B:876:ILE:HD11	1.92	0.51
1:D:186:ASP:O	1:D:190:VAL:HG23	2.10	0.51
1:D:698:LYS:H	1:D:771:HIS:HB2	1.76	0.51
1:A:460:MET:HB3	1:A:485:CYS:HA	1.92	0.51
1:A:700:ILE:O	1:A:704:ILE:HG12	2.11	0.51
1:B:167:ARG:NH2	1:B:180:GLU:OE1	2.42	0.51
1:C:143:ASN:HB3	1:C:146:LYS:HB2	1.92	0.51
1:B:350:HIS:NE2	1:B:352:THR:OG1	2.44	0.50
1:B:827:ILE:HD12	1:B:830:MET:HG3	1.93	0.50
1:C:160:PHE:HA	1:C:163:TYR:CE1	2.46	0.50
1:C:405:VAL:HG11	1:C:443:ARG:HG3	1.92	0.50
1:C:982:LEU:HD13	1:C:991:GLY:HA3	1.93	0.50
1:B:21:MET:SD	1:B:21:MET:N	2.82	0.50
1:B:30:MET:HE1	1:B:33:PHE:HB3	1.93	0.50
1:D:700:ILE:O	1:D:704:ILE:HG12	2.11	0.50
1:C:692:PHE:HD1	1:C:743:ALA:HA	1.76	0.50
1:B:496:GLN:HB3	1:B:503:LEU:HD23	1.93	0.50
1:B:964:SER:OG	1:B:965:THR:N	2.45	0.50
1:D:597:PHE:HD2	1:D:605:VAL:HG13	1.77	0.50
1:D:134:SER:HB2	1:D:254:HIS:HE1	1.77	0.50
1:D:218:SER:HB2	1:D:236:VAL:HG22	1.93	0.50
1:A:270:GLN:HB3	1:A:272:LEU:HD23	1.94	0.50
1:A:423:LEU:HD12	1:A:924:MET:HE2	1.94	0.50
1:A:687:ASP:N	1:A:692:PHE:O	2.45	0.50
1:D:491:LEU:HD22	1:D:737:LEU:HB2	1.94	0.49
1:D:233:ILE:O	1:D:237:ASN:ND2	2.45	0.49
1:A:140:SER:OG	1:A:141:CYS:N	2.45	0.49
1:A:297:THR:HG23	1:A:300:GLY:H	1.78	0.49
1:C:21:MET:O	1:C:25:PHE:N	2.42	0.49
1:C:989:ASP:OD1	1:C:989:ASP:N	2.45	0.49
1:B:729:SER:O	1:B:765:ARG:NH2	2.36	0.49
1:A:120:PHE:HE1	1:A:214:LEU:HA	1.76	0.49
1:C:597:PHE:CD2	1:C:605:VAL:HG13	2.47	0.49
1:D:519:ILE:HB	1:D:526:LYS:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:142:GLN:HG2	1:D:202:SER:HB3	1.95	0.49
1:A:789:LEU:HD13	1:A:827:ILE:HD13	1.95	0.49
1:C:755:VAL:HG12	1:C:777:SER:HB2	1.95	0.49
1:B:358:ASN:HA	1:B:361:LYS:HG2	1.95	0.49
1:B:833:ASP:OD1	1:B:833:ASP:N	2.43	0.49
1:D:692:PHE:HD1	1:D:743:ALA:HA	1.77	0.49
1:C:457:ILE:HD13	1:C:927:THR:HG23	1.93	0.48
1:A:829:SER:HB2	1:D:473:PRO:HG3	1.94	0.48
1:C:1010:LEU:HD23	1:C:1052:LEU:HD12	1.95	0.48
1:B:351:ILE:HD11	1:B:379:HIS:HB2	1.95	0.48
1:A:304:MET:O	1:A:308:ILE:HG12	2.14	0.48
1:C:138:ILE:O	1:C:202:SER:OG	2.31	0.48
1:C:578:ARG:NH2	1:C:948:GLU:OE2	2.37	0.48
1:D:308:ILE:HA	1:D:312:LEU:HD23	1.95	0.48
1:A:205:GLY:HA3	1:A:255:LEU:HD12	1.95	0.48
1:C:746:PHE:HD1	1:C:976:ARG:HH11	1.62	0.48
1:B:512:SER:OG	1:B:514:ARG:NH1	2.46	0.48
1:A:508:ALA:HB1	1:A:919:VAL:HG11	1.96	0.48
1:C:364:LEU:HD11	1:C:397:GLN:HE21	1.77	0.48
1:C:208:PHE:CE2	1:C:248:THR:HA	2.49	0.48
1:B:380:ASN:O	1:B:402:GLN:NE2	2.46	0.48
1:B:402:GLN:O	1:B:413:ARG:NH2	2.47	0.48
1:B:692:PHE:HZ	1:B:944:GLY:HA3	1.78	0.48
1:D:457:ILE:HD13	1:D:927:THR:HG23	1.96	0.48
1:A:807:GLN:HG3	1:A:883:VAL:HG11	1.95	0.47
1:A:888:VAL:HA	1:A:891:LEU:HD23	1.95	0.47
1:C:321:GLU:HA	1:C:324:GLU:HG2	1.96	0.47
1:B:210:ARG:HB2	1:B:213:ARG:HH21	1.79	0.47
1:A:186:ASP:HA	1:A:189:THR:HG22	1.95	0.47
1:A:563:LEU:HD11	1:A:599:ALA:HB2	1.95	0.47
1:C:207:ARG:O	1:C:207:ARG:NH1	2.45	0.47
1:C:901:THR:HB	1:C:905:LEU:HD11	1.96	0.47
1:A:534:ASN:HD21	1:A:1036:ASN:HD22	1.62	0.47
1:C:606:LYS:O	1:C:606:LYS:NZ	2.47	0.47
1:C:921:ASP:N	1:C:921:ASP:OD1	2.47	0.47
1:A:158:VAL:HA	1:A:161:LEU:HD12	1.95	0.47
1:A:511:PHE:O	1:A:922:SER:OG	2.30	0.47
1:A:833:ASP:OD1	1:A:833:ASP:N	2.46	0.47
1:C:690:GLY:HA3	1:C:968:THR:HB	1.95	0.47
1:B:190:VAL:HB	1:B:191:PRO:HD3	1.97	0.47
1:B:335:SER:HA	1:B:413:ARG:HG3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1051:CYS:SG	1:C:1052:LEU:N	2.88	0.47
1:B:280:LEU:HD11	1:B:293:VAL:HG23	1.97	0.47
1:D:20:ARG:HD3	1:D:266:PHE:CE2	2.50	0.47
1:D:221:LEU:HB3	1:D:226:ILE:HD12	1.97	0.47
1:D:561:LEU:HD23	1:D:607:ARG:HB3	1.96	0.47
1:A:191:PRO:HA	1:A:194:PHE:HB2	1.96	0.47
1:C:790:ARG:HH21	1:C:830:MET:HE3	1.80	0.47
1:D:226:ILE:HG22	1:D:228:LYS:HE3	1.97	0.47
1:A:278:VAL:O	1:A:281:LEU:HG	2.15	0.46
1:C:159:PHE:HA	1:C:162:LEU:HG	1.96	0.46
1:B:369:ASP:OD1	1:B:369:ASP:N	2.45	0.46
1:B:700:ILE:O	1:B:704:ILE:HG12	2.16	0.46
1:D:206:LEU:HD21	1:D:209:LEU:HD13	1.97	0.46
1:A:964:SER:OG	1:A:965:THR:N	2.48	0.46
1:C:992:ASP:N	1:C:992:ASP:OD1	2.48	0.46
1:B:1007:TYR:HB2	1:B:1009:MET:HE1	1.97	0.46
1:A:362:ASP:O	1:A:368:ARG:NH1	2.39	0.46
1:A:1009:MET:HE2	1:A:1009:MET:HA	1.98	0.46
1:C:410:ASP:O	1:C:414:VAL:HG23	2.16	0.46
1:D:491:LEU:HD12	1:D:736:ASN:HB3	1.98	0.46
1:D:931:ASP:N	1:D:931:ASP:OD1	2.49	0.46
1:A:485:CYS:SG	1:A:488:GLU:HB3	2.56	0.46
1:B:976:ARG:HA	1:B:1051:CYS:HA	1.97	0.46
1:A:697:PRO:HB3	1:A:771:HIS:HD2	1.81	0.46
1:C:185:VAL:HG21	1:C:209:LEU:HD13	1.97	0.46
1:B:110:LEU:HD13	1:B:113:ARG:HH21	1.80	0.46
1:D:130:TYR:HD1	1:D:207:ARG:HB3	1.79	0.46
1:A:749:HIS:CD2	1:A:749:HIS:H	2.34	0.46
1:C:498:CYS:HA	1:C:799:MET:HG2	1.98	0.46
1:B:937:ILE:O	1:B:941:VAL:HG22	2.16	0.46
1:A:27:ALA:HA	1:A:31:VAL:HB	1.97	0.46
1:A:503:LEU:HA	1:A:506:MET:HB3	1.97	0.46
1:C:889:GLN:HB2	1:C:897:ASP:HB3	1.98	0.46
1:A:186:ASP:O	1:A:190:VAL:HG22	2.16	0.46
1:A:460:MET:HE3	1:A:465:ASN:HB2	1.97	0.45
1:D:122:LEU:HD22	1:D:152:ILE:HG21	1.98	0.45
1:A:206:LEU:HD12	1:A:255:LEU:HD11	1.98	0.45
1:A:246:TRP:HD1	1:A:247:LEU:HD22	1.82	0.45
1:B:176:TRP:HA	1:B:179:LEU:HB2	1.98	0.45
1:B:971:ASN:H	1:B:1056:ASP:HB2	1.80	0.45
1:B:974:ARG:NH1	1:B:1053:MET:SD	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:VAL:HA	1:A:184:VAL:HG22	1.99	0.45
1:A:555:GLU:HB3	1:A:1004:LEU:HD12	1.99	0.45
1:A:1003:ALA:HB1	1:A:1009:MET:HB3	1.97	0.45
1:A:495:ALA:HB2	1:A:737:LEU:HD12	1.98	0.45
1:A:568:ILE:HG22	1:A:595:GLY:HA2	1.98	0.45
1:D:21:MET:SD	1:D:203:TRP:NE1	2.89	0.45
1:A:369:ASP:OD1	1:A:370:ASP:N	2.49	0.45
1:A:528:TYR:HE2	1:A:905:LEU:HA	1.82	0.45
1:D:378:LEU:HD11	1:D:414:VAL:HG21	1.98	0.45
1:A:438:ALA:O	1:A:442:MET:HG2	2.17	0.45
1:A:889:GLN:O	1:D:449:ASN:ND2	2.46	0.45
1:C:460:MET:HE1	1:C:465:ASN:HB2	1.97	0.45
1:C:146:LYS:HD3	1:C:146:LYS:HA	1.77	0.45
1:C:383:PRO:HB3	1:C:387:LEU:HD23	1.99	0.45
1:C:208:PHE:HE2	1:C:248:THR:HA	1.82	0.45
1:D:530:GLU:O	1:D:533:SER:OG	2.33	0.44
1:C:423:LEU:HD13	1:C:457:ILE:HB	1.98	0.44
1:B:301:ARG:HA	1:B:304:MET:HG3	1.98	0.44
1:D:207:ARG:HG3	1:D:210:ARG:HH11	1.82	0.44
1:A:122:LEU:HD12	1:A:122:LEU:HA	1.78	0.44
1:A:425:LEU:HD22	1:A:924:MET:HE1	1.99	0.44
1:C:744:SER:HB3	1:C:972:ARG:HG2	1.98	0.44
1:B:142:GLN:HG3	1:B:150:LEU:HD13	1.98	0.44
1:D:358:ASN:HA	1:D:361:LYS:HG2	1.98	0.44
1:B:687:ASP:OD2	1:B:689:THR:OG1	2.35	0.44
1:D:20:ARG:NH2	1:D:22:TRP:HB2	2.33	0.44
1:D:448:LYS:HE2	1:D:456:ILE:HG13	2.00	0.44
1:D:921:ASP:OD1	1:D:921:ASP:N	2.49	0.44
1:A:131:PHE:O	1:A:135:SER:OG	2.29	0.44
1:A:257:GLU:OE2	1:A:272:LEU:N	2.46	0.44
1:A:185:VAL:HG21	1:A:212:LEU:HD22	1.98	0.44
1:B:438:ALA:HB1	1:D:818:LYS:HB3	1.99	0.44
1:D:441:ILE:O	1:D:445:ILE:HG12	2.18	0.44
1:D:756:PHE:HB3	1:D:763:LEU:HD21	1.99	0.44
1:A:880:THR:HG21	1:A:891:LEU:HD11	1.99	0.44
1:B:261:ASP:HB2	1:B:264:GLU:HB2	2.00	0.44
1:B:735:ARG:HE	1:B:769:THR:HG1	1.60	0.44
1:C:541:LEU:HD12	1:C:545:PHE:HD2	1.83	0.44
1:C:907:GLN:HE21	1:C:1018:ARG:HD3	1.83	0.44
1:C:965:THR:OG1	1:C:967:GLN:O	2.25	0.44
1:B:138:ILE:HG23	1:B:204:LEU:HB2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:236:VAL:HA	1:C:239:LEU:HG	2.00	0.43
1:C:300:GLY:O	1:C:304:MET:HG2	2.18	0.43
1:C:454:ILE:HG23	1:C:456:ILE:HD11	2.00	0.43
1:B:536:MET:HE1	1:B:566:ILE:HD12	1.98	0.43
1:B:545:PHE:CZ	1:B:557:CYS:HB3	2.53	0.43
1:C:304:MET:HE2	1:C:307:PHE:HE2	1.83	0.43
1:C:281:LEU:O	1:C:284:THR:OG1	2.28	0.43
1:C:330:LYS:HE3	1:C:402:GLN:HG2	2.01	0.43
1:B:807:GLN:HB2	1:B:883:VAL:HG11	2.00	0.43
1:D:992:ASP:HA	1:D:1045:PRO:HG3	2.00	0.43
1:D:1018:ARG:NH2	1:D:1028:CYS:SG	2.92	0.43
1:C:415:LYS:HB3	1:C:415:LYS:HE2	1.82	0.43
1:C:496:GLN:HG3	1:C:941:VAL:HG23	1.99	0.43
1:B:378:LEU:HD21	1:B:414:VAL:HG21	2.00	0.43
1:D:282:MET:HA	1:D:282:MET:HE2	2.00	0.43
1:D:506:MET:HE1	1:D:1035:THR:HA	2.00	0.43
1:A:236:VAL:HA	1:A:239:LEU:HG	2.00	0.43
1:A:428:LYS:HA	1:A:461:LEU:HD21	2.00	0.43
1:C:735:ARG:HA	1:C:770:LEU:HD21	2.01	0.43
1:C:125:GLY:HA3	1:C:156:PHE:HZ	1.83	0.43
1:C:149:THR:O	1:C:153:ASP:N	2.49	0.43
1:C:370:ASP:OD1	1:C:370:ASP:N	2.49	0.43
1:B:1048:LEU:HD11	1:B:1050:PHE:HD2	1.82	0.43
1:C:700:ILE:O	1:C:704:ILE:HG12	2.18	0.43
1:A:441:ILE:HG21	1:C:822:LEU:HD21	2.00	0.43
1:A:827:ILE:HD12	1:A:830:MET:HG3	1.99	0.43
1:C:253:ILE:HA	1:C:256:VAL:HG22	2.00	0.43
1:D:119:VAL:HB	1:D:213:ARG:HD2	1.99	0.43
1:B:297:THR:HB	1:B:299:LEU:HD23	2.00	0.43
1:D:249:ALA:O	1:D:253:ILE:HG23	2.18	0.43
1:C:235:LEU:HD23	1:C:239:LEU:HD23	2.00	0.43
1:B:554:CYS:SG	1:B:565:MET:HE1	2.59	0.43
1:A:351:ILE:HG12	1:A:379:HIS:HD2	1.84	0.42
1:A:442:MET:HE3	1:A:442:MET:HB3	1.85	0.42
1:A:830:MET:HE3	1:A:830:MET:HB3	1.91	0.42
1:D:460:MET:HE1	1:D:465:ASN:HB2	2.01	0.42
1:B:378:LEU:HD11	1:B:414:VAL:HG21	2.01	0.42
1:D:20:ARG:HH21	1:D:22:TRP:HB2	1.84	0.42
1:B:799:MET:SD	1:B:879:ILE:HG22	2.59	0.42
1:A:496:GLN:HG3	1:A:941:VAL:HA	2.01	0.42
1:C:726:ASP:OD1	1:C:726:ASP:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:937:ILE:O	1:C:941:VAL:HG12	2.19	0.42
1:B:568:ILE:HG22	1:B:595:GLY:HA2	2.01	0.42
1:B:739:MET:HB3	1:B:740:PRO:HD3	2.02	0.42
1:A:221:LEU:HD21	1:A:227:LEU:HB2	2.02	0.42
1:A:692:PHE:HE1	1:A:943:GLY:HA3	1.84	0.42
1:C:353:LEU:HD12	1:C:387:LEU:HB2	2.02	0.42
1:B:902:GLU:OE1	1:B:903:LEU:N	2.52	0.42
1:D:742:ARG:HD2	1:D:774:PRO:HD2	2.01	0.42
1:D:902:GLU:HG3	1:D:904:TYR:CE2	2.55	0.42
1:C:301:ARG:HB2	1:B:279:TYR:CD1	2.54	0.42
1:A:122:LEU:HD11	1:A:156:PHE:CD1	2.54	0.42
1:B:425:LEU:HD22	1:B:924:MET:HE1	2.01	0.42
1:D:127:LEU:HD23	1:D:127:LEU:HA	1.88	0.42
1:D:232:SER:O	1:D:236:VAL:HG23	2.19	0.42
1:D:699:GLU:OE1	1:D:702:LYS:NZ	2.51	0.42
1:D:989:ASP:OD1	1:D:989:ASP:N	2.52	0.42
1:D:1026:SER:OG	1:D:1027:GLN:N	2.52	0.42
1:A:196:SER:HB2	1:A:207:ARG:HH21	1.84	0.42
1:B:304:MET:HA	1:B:307:PHE:HB3	2.00	0.42
1:B:597:PHE:HD2	1:B:605:VAL:HG13	1.85	0.42
1:D:299:LEU:HA	1:D:302:LEU:HD12	2.01	0.42
1:D:511:PHE:HZ	1:D:937:ILE:HD11	1.84	0.42
1:D:937:ILE:HD13	1:D:937:ILE:HA	1.83	0.42
1:A:946:THR:OG1	1:A:949:LEU:HD23	2.19	0.42
1:B:423:LEU:HD12	1:B:924:MET:HE2	2.01	0.42
1:B:511:PHE:CZ	1:B:937:ILE:HD11	2.54	0.42
1:D:931:ASP:OD1	1:D:932:ASN:ND2	2.53	0.42
1:A:229:THR:HG23	1:A:232:SER:H	1.84	0.42
1:C:261:ASP:OD2	1:C:268:ASN:ND2	2.38	0.42
1:A:319:VAL:HA	1:A:322:ILE:HG12	2.02	0.41
1:D:707:ARG:NE	1:D:788:ASP:OD1	2.52	0.41
1:D:722:CYS:HB3	1:D:783:PRO:HB3	2.02	0.41
1:D:1044:VAL:HG12	1:D:1046:THR:H	1.83	0.41
1:A:442:MET:HA	1:A:445:ILE:HG22	2.02	0.41
1:C:163:TYR:OH	1:C:213:ARG:NH2	2.53	0.41
1:B:207:ARG:O	1:B:210:ARG:NH2	2.53	0.41
1:B:1002:LYS:HD3	1:B:1002:LYS:HA	1.77	0.41
1:D:134:SER:HB2	1:D:254:HIS:CE1	2.55	0.41
1:D:612:CYS:SG	1:D:613:LYS:N	2.93	0.41
1:A:795:ASN:HA	1:A:876:ILE:HD11	2.02	0.41
1:A:817:ASP:O	1:A:821:ILE:HG12	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:MET:SD	1:C:1035:THR:OG1	2.65	0.41
1:C:567:ALA:HB2	1:C:581:ILE:HD13	2.01	0.41
1:B:693:HIS:CE1	1:B:744:SER:HA	2.56	0.41
1:D:496:GLN:NE2	1:D:940:LEU:O	2.52	0.41
1:D:950:GLU:HA	1:D:953:ILE:HG22	2.02	0.41
1:C:700:ILE:HB	1:C:767:TRP:CD1	2.55	0.41
1:B:167:ARG:HA	1:B:167:ARG:HD2	1.80	0.41
1:B:723:ILE:HD11	1:B:756:PHE:HD2	1.85	0.41
1:B:895:ASP:OD1	1:B:895:ASP:N	2.51	0.41
1:D:1033:VAL:HG23	1:D:1050:PHE:HE2	1.85	0.41
1:B:706:THR:HG22	1:B:709:GLU:HG2	2.02	0.41
1:B:876:ILE:HD13	1:B:876:ILE:HA	1.92	0.41
1:D:320:PRO:O	1:D:323:ILE:HG22	2.20	0.41
1:A:172:ASN:HB3	1:A:173:ASP:H	1.71	0.41
1:C:699:GLU:HG3	1:C:701:GLU:H	1.85	0.41
1:C:811:ASP:OD1	1:C:811:ASP:N	2.54	0.41
1:A:386:GLU:O	1:A:390:LEU:HG	2.20	0.41
1:C:350:HIS:CE1	1:C:352:THR:HG1	2.39	0.41
1:D:300:GLY:O	1:D:304:MET:HG2	2.20	0.41
1:D:496:GLN:HE21	1:D:941:VAL:HA	1.85	0.41
1:A:490:LYS:HG3	1:A:915:PHE:HE2	1.85	0.41
1:A:692:PHE:HD1	1:A:743:ALA:HA	1.86	0.41
1:C:122:LEU:HB3	1:C:210:ARG:HH11	1.86	0.41
1:C:237:ASN:O	1:C:241:ILE:HG23	2.21	0.41
1:B:442:MET:HA	1:B:445:ILE:HG22	2.03	0.41
1:D:992:ASP:N	1:D:992:ASP:OD1	2.49	0.41
1:A:604:GLU:OE2	1:A:607:ARG:NH1	2.42	0.41
1:C:295:ALA:HB2	1:C:304:MET:HE3	2.03	0.41
1:C:335:SER:OG	1:C:336:TYR:N	2.53	0.41
1:B:441:ILE:HG21	1:D:822:LEU:HD11	2.03	0.41
1:D:122:LEU:HG	1:D:125:GLY:HA3	2.03	0.41
1:A:159:PHE:O	1:A:162:LEU:HG	2.21	0.40
1:D:726:ASP:N	1:D:726:ASP:OD1	2.52	0.40
1:C:210:ARG:HA	1:C:213:ARG:HB2	2.03	0.40
1:C:804:SER:OG	1:C:807:GLN:HB3	2.21	0.40
1:C:1033:VAL:HG23	1:C:1050:PHE:HE2	1.85	0.40
1:B:384:ASN:O	1:B:387:LEU:N	2.53	0.40
1:D:26:LEU:HD22	1:D:26:LEU:HA	1.91	0.40
1:D:735:ARG:HA	1:D:770:LEU:HD21	2.02	0.40
1:A:351:ILE:HD11	1:A:379:HIS:HB2	2.03	0.40
1:B:164:PHE:HE1	1:B:187:PHE:CE1	2.40	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:ARG:HB3	1:B:177:PHE:HE1	1.87	0.40
1:B:330:LYS:HA	1:B:330:LYS:HD2	1.87	0.40
1:B:511:PHE:CE2	1:B:937:ILE:HD11	2.55	0.40
1:D:246:TRP:HZ2	1:D:282:MET:HB2	1.86	0.40
1:A:529:LEU:HA	1:A:532:VAL:HG12	2.02	0.40
1:A:1056:ASP:OD1	1:A:1056:ASP:N	2.46	0.40
1:B:292:ASP:N	1:B:292:ASP:OD1	2.53	0.40
1:B:347:VAL:HG22	1:B:423:LEU:HB2	2.03	0.40
1:B:526:LYS:HB3	1:B:526:LYS:HE2	1.91	0.40
1:D:563:LEU:HD21	1:D:597:PHE:CG	2.57	0.40
1:C:216:GLN:O	1:C:219:GLU:HG2	2.22	0.40
1:B:872:THR:HG23	1:B:874:VAL:HG12	2.02	0.40
1:B:1017:LEU:HG	1:B:1031:ARG:HE	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	803/1072 (75%)	750 (93%)	53 (7%)	0	100	100
1	B	803/1072 (75%)	761 (95%)	42 (5%)	0	100	100
1	C	843/1072 (79%)	805 (96%)	38 (4%)	0	100	100
1	D	838/1072 (78%)	796 (95%)	42 (5%)	0	100	100
All	All	3287/4288 (77%)	3112 (95%)	175 (5%)	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	724/943 (77%)	723 (100%)	1 (0%)	88	90
1	B	726/943 (77%)	725 (100%)	1 (0%)	88	90
1	C	750/943 (80%)	749 (100%)	1 (0%)	88	90
1	D	747/943 (79%)	747 (100%)	0	100	100
All	All	2947/3772 (78%)	2944 (100%)	3 (0%)	87	90

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	128	VAL
1	C	128	VAL
1	B	329	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (48) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	157	ASN
1	A	182	ASN
1	A	200	ASN
1	A	222	GLN
1	A	231	ASN
1	A	258	ASN
1	A	397	GLN
1	A	462	GLN
1	A	468	HIS
1	A	745	ASN
1	A	749	HIS
1	A	816	GLN
1	A	893	GLN
1	A	967	GLN
1	A	971	ASN
1	A	1036	ASN

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Mol	Chain	Res	Type
1	C	142	GLN
1	C	172	ASN
1	C	449	ASN
1	C	462	GLN
1	C	464	HIS
1	C	525	GLN
1	C	534	ASN
1	C	907	GLN
1	B	216	GLN
1	B	344	HIS
1	B	380	ASN
1	B	465	ASN
1	B	468	HIS
1	B	496	GLN
1	B	509	ASN
1	B	808	ASN
1	B	893	GLN
1	B	907	GLN
1	B	971	ASN
1	B	1054	GLN
1	D	216	GLN
1	D	225	ASN
1	D	267	GLN
1	D	465	ASN
1	D	534	ASN
1	D	693	HIS
1	D	745	ASN
1	D	807	GLN
1	D	808	ASN
1	D	907	GLN
1	D	932	ASN
1	D	971	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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.

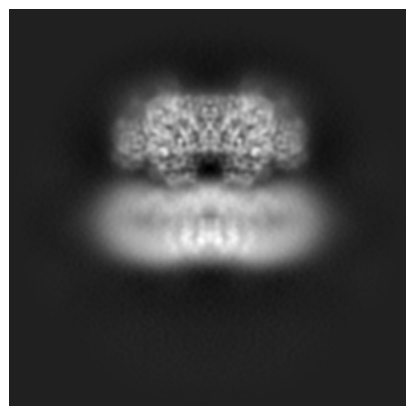
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-40045. These allow visual inspection of the internal detail of the map and identification of artifacts.

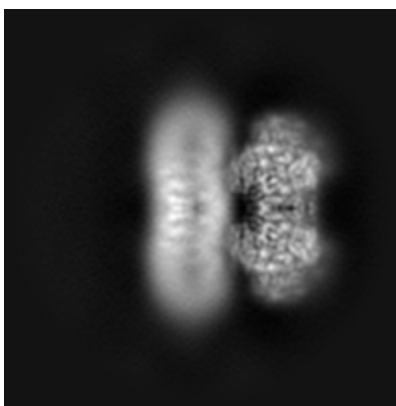
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

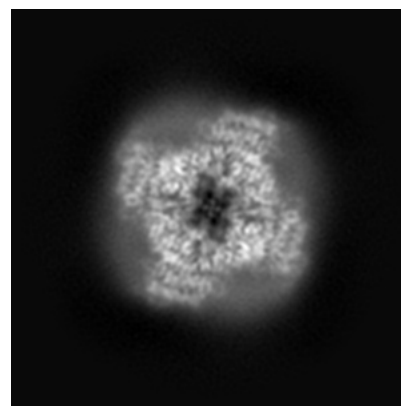
6.1.1 Primary map



X

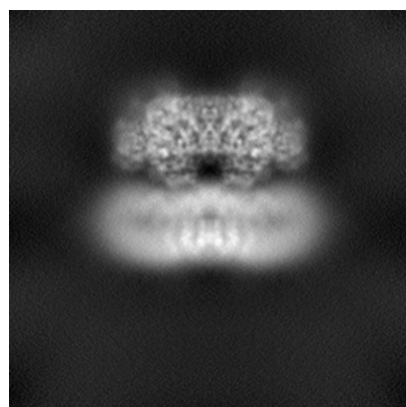


Y

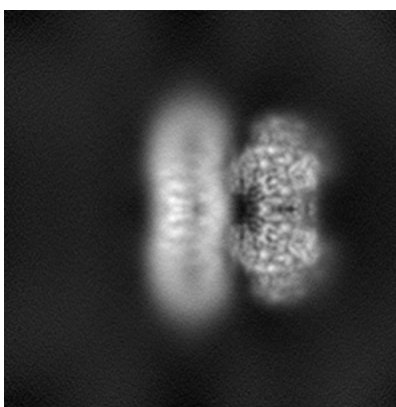


Z

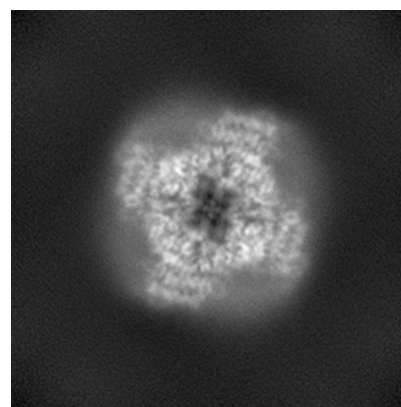
6.1.2 Raw map



X



Y

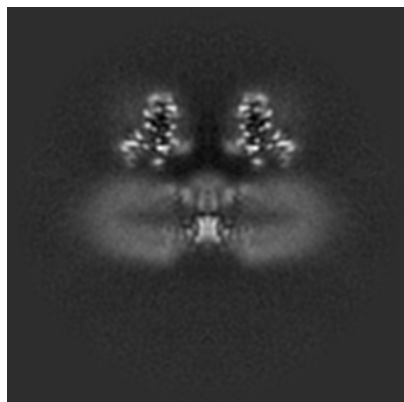


Z

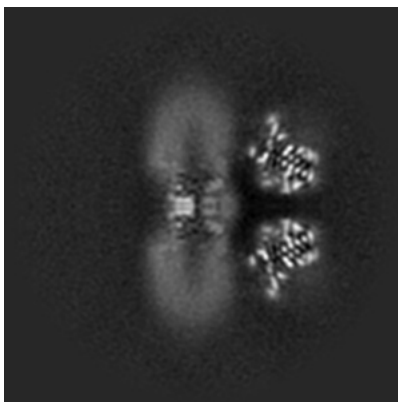
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

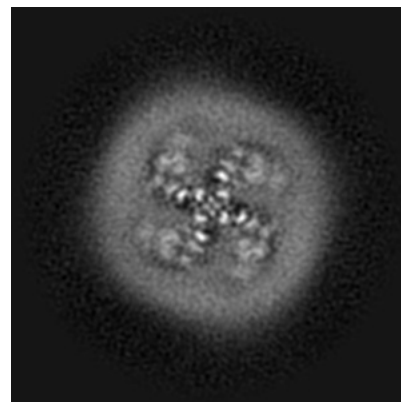
6.2.1 Primary map



X Index: 128

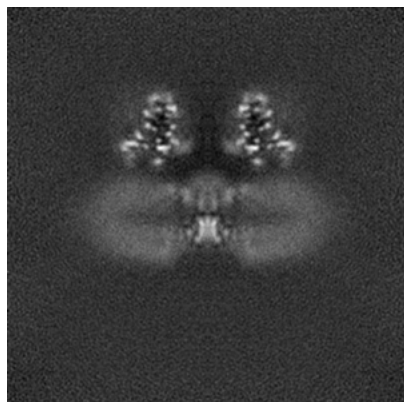


Y Index: 128

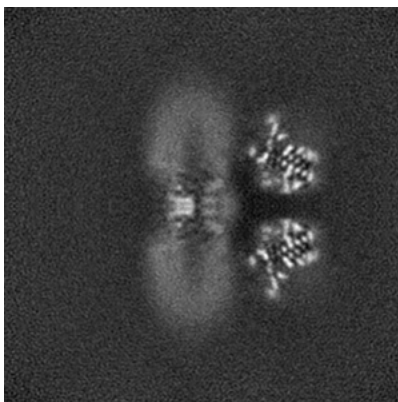


Z Index: 128

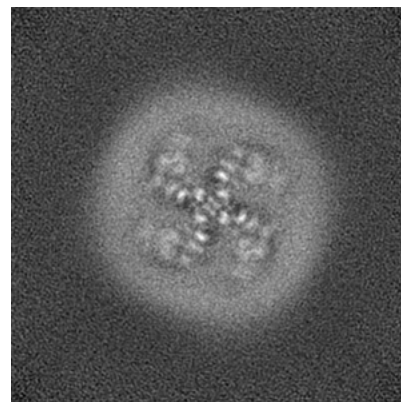
6.2.2 Raw map



X Index: 128



Y Index: 128

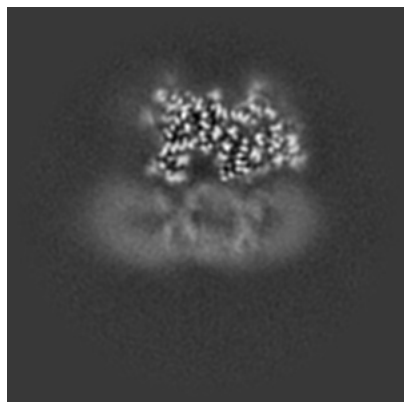


Z Index: 128

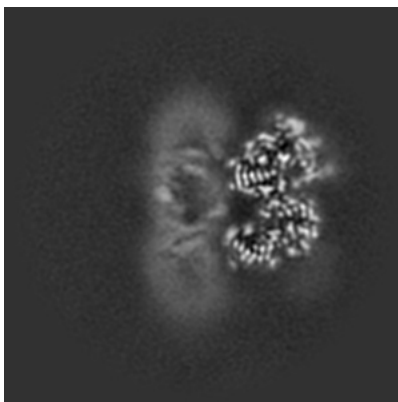
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

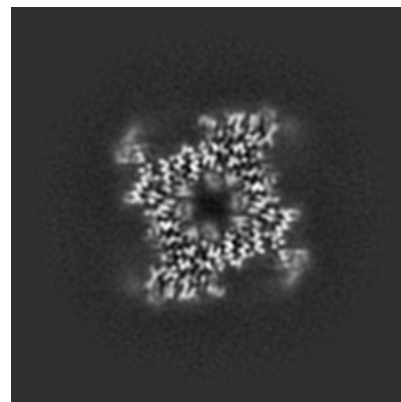
6.3.1 Primary map



X Index: 156

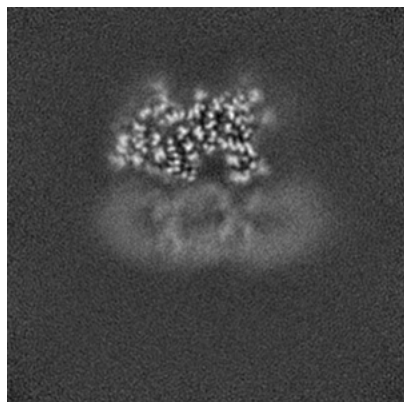


Y Index: 105

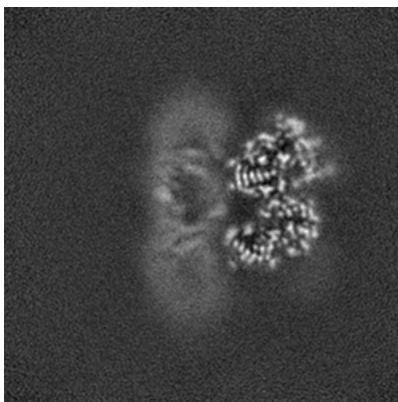


Z Index: 166

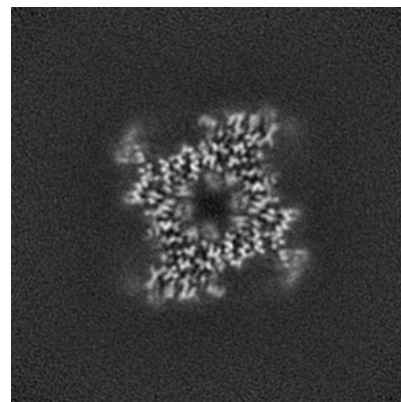
6.3.2 Raw map



X Index: 100



Y Index: 105

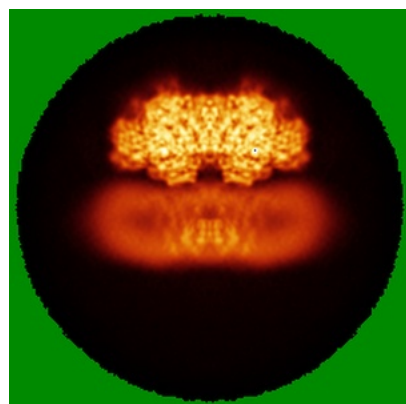


Z Index: 166

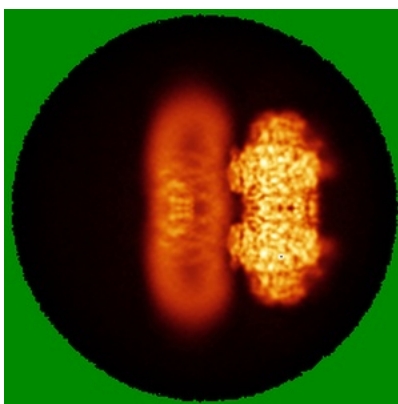
The images above show the largest variance slices of the map in three orthogonal directions.

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

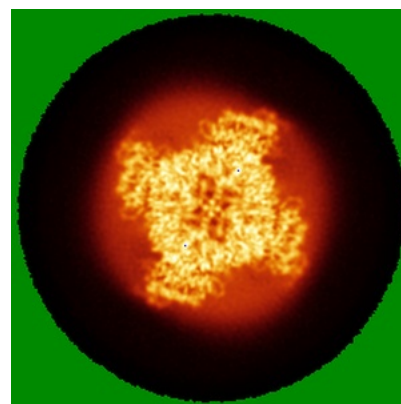
6.4.1 Primary map



X

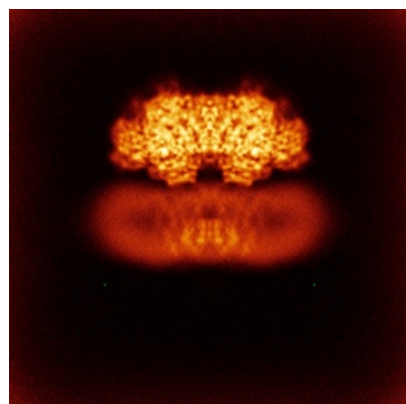


Y

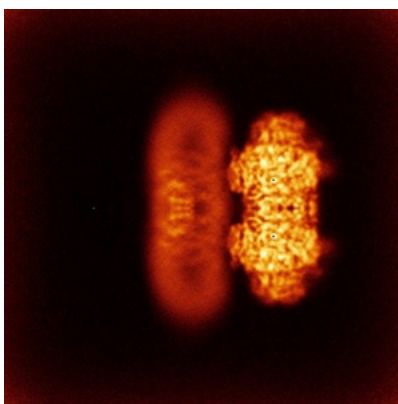


Z

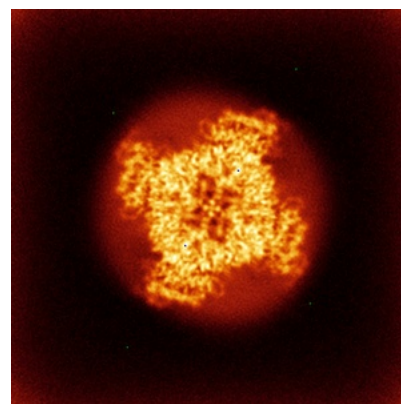
6.4.2 Raw map



X



Y

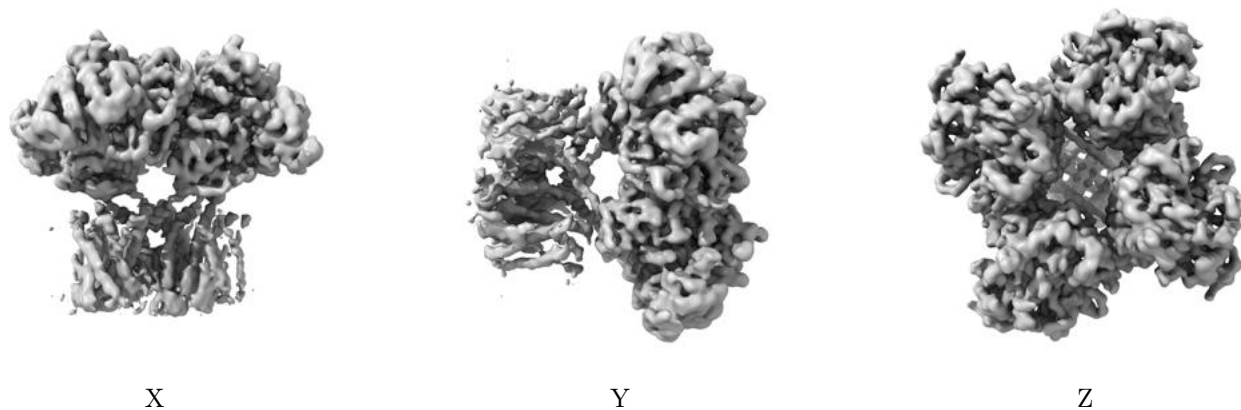


Z

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.

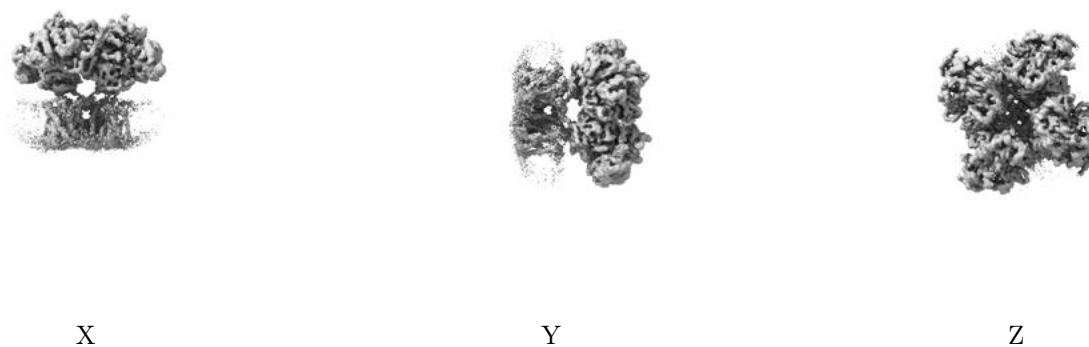
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.28. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



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

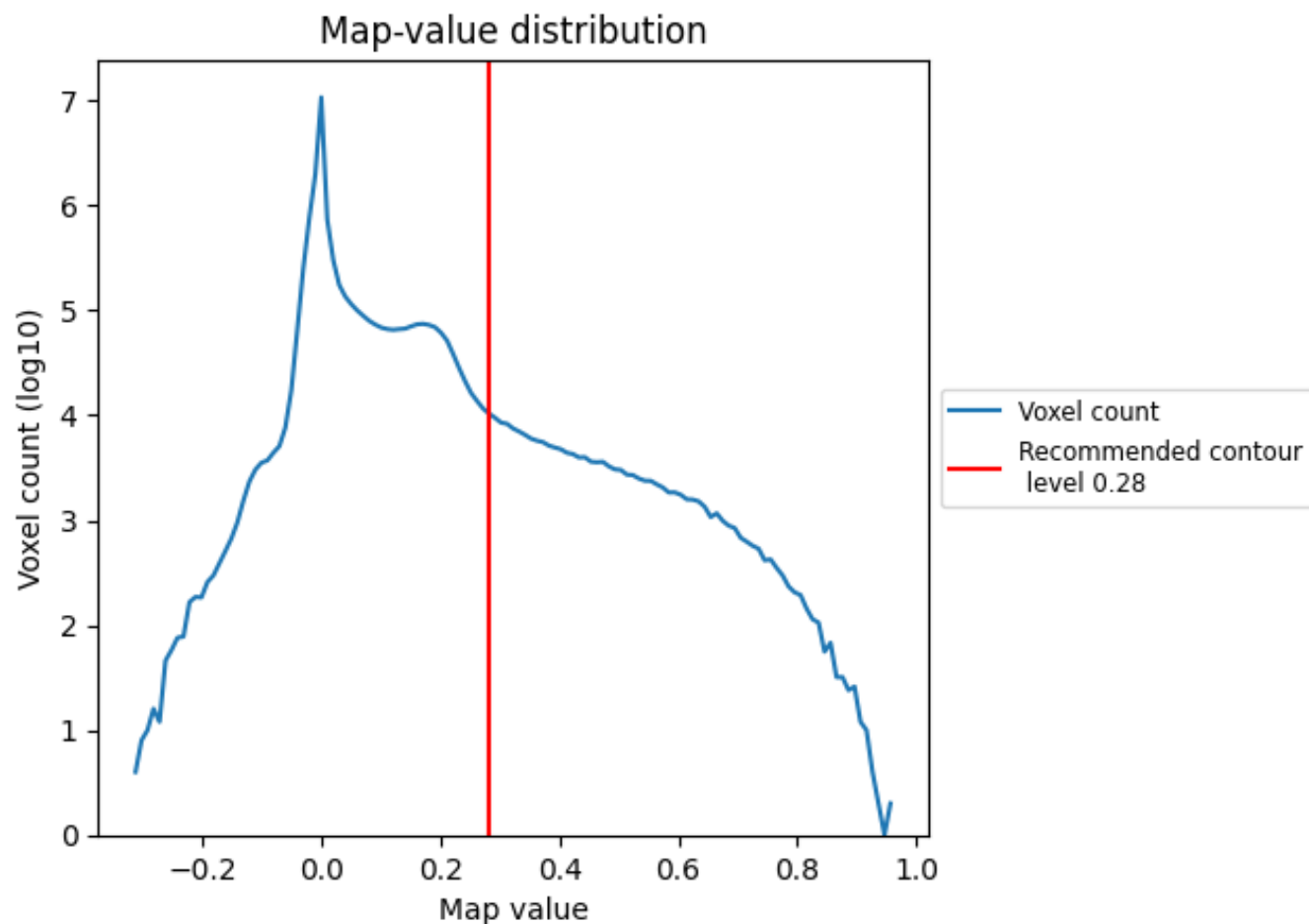
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

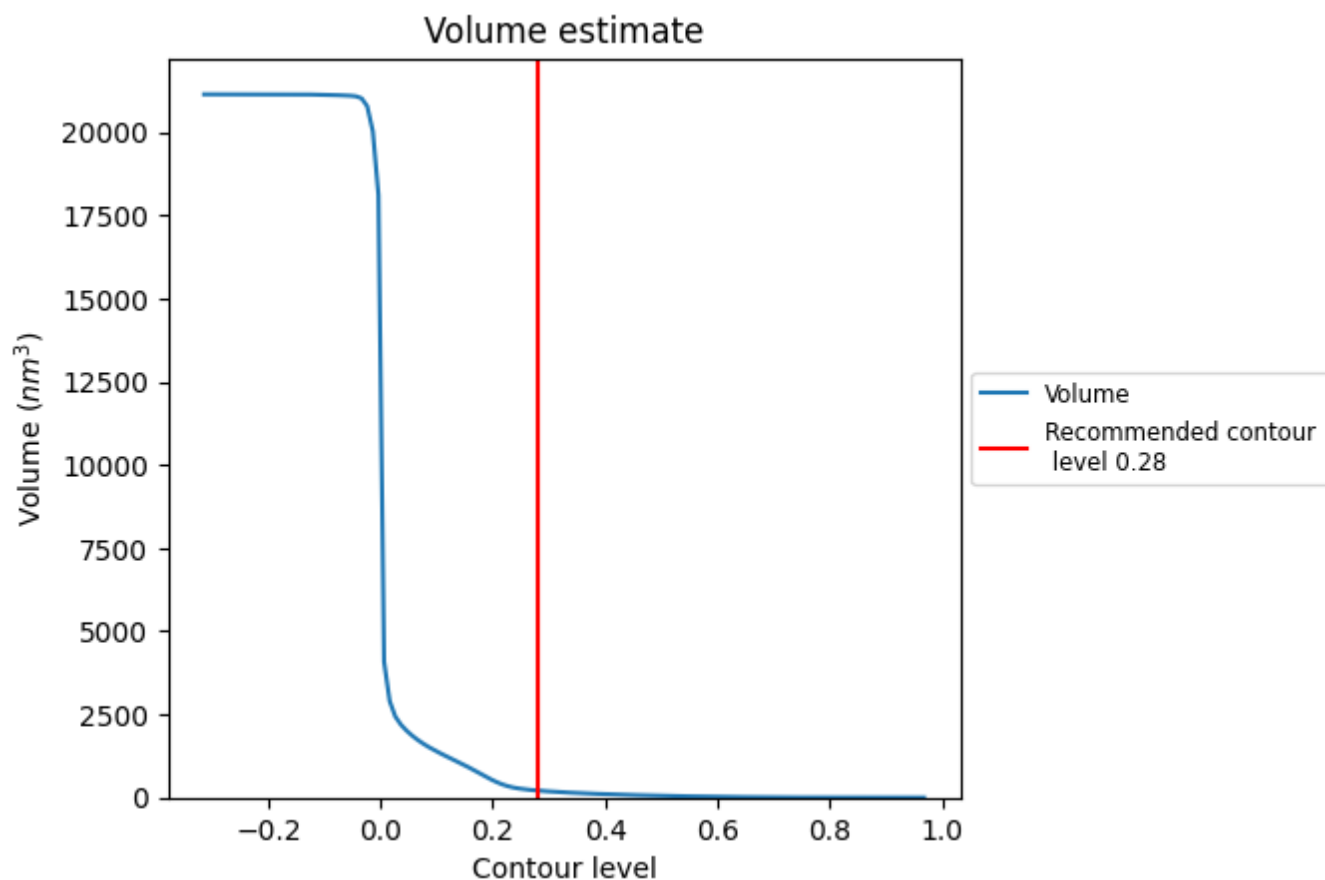
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

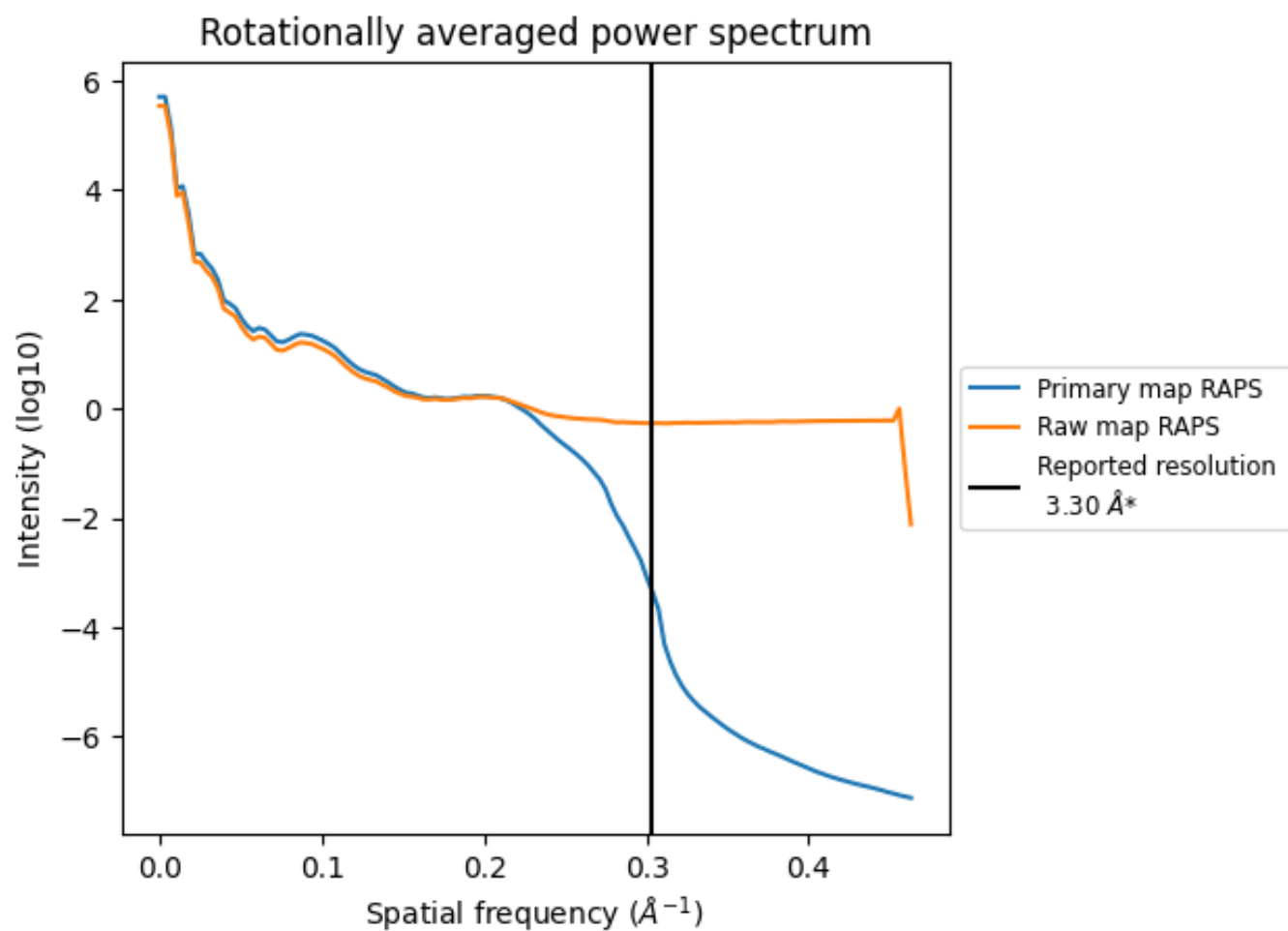
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 210 nm³; this corresponds to an approximate mass of 190 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 ⓘ

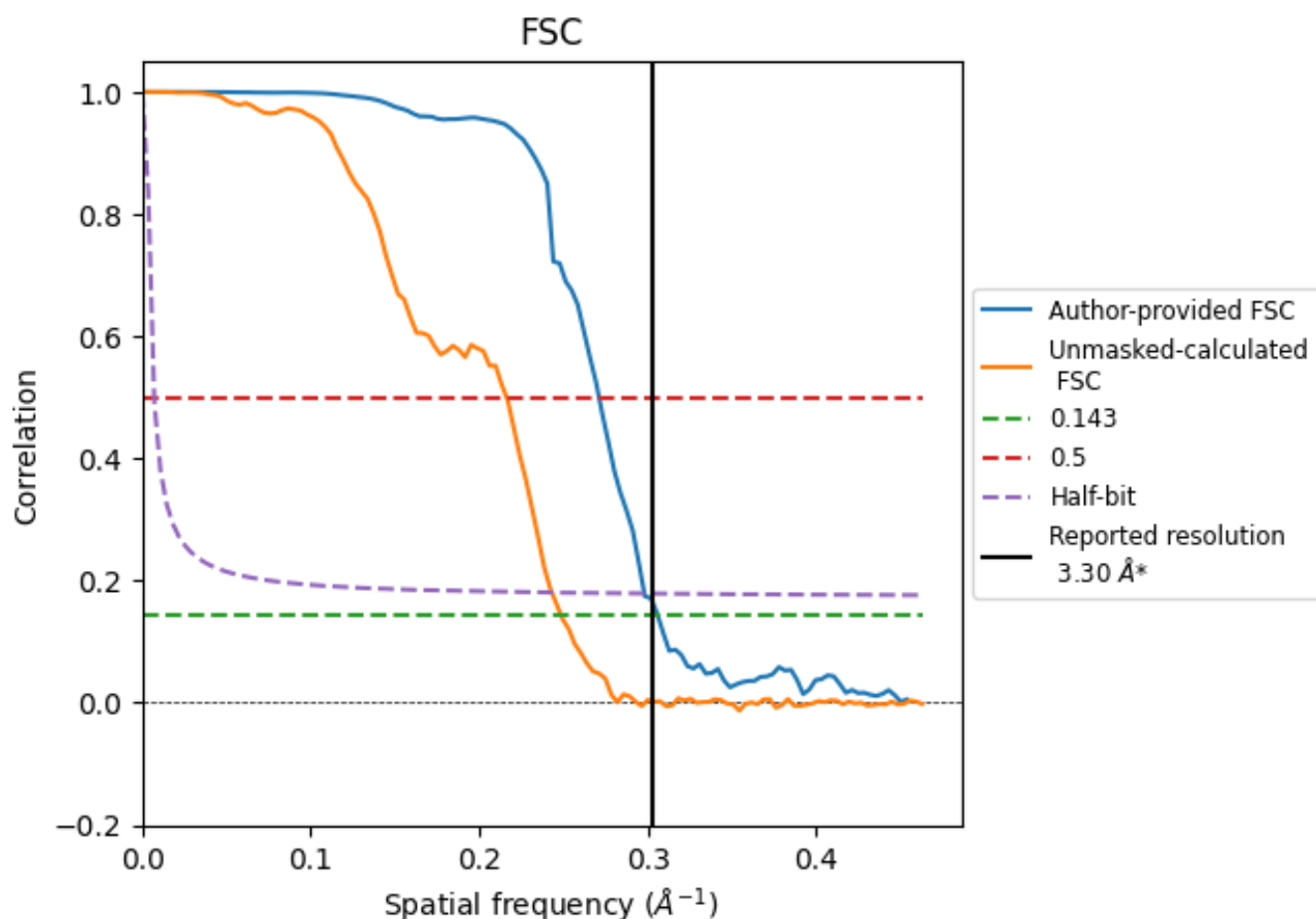


*Reported resolution corresponds to spatial frequency of 0.303 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of $0.303 \text{ \AA}^{-1}$

8.2 Resolution estimates [i](#)

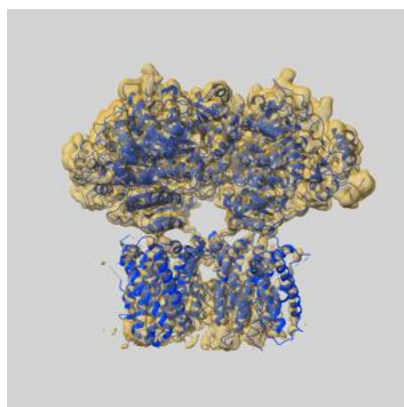
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	3.27	3.69	3.35
Unmasked-calculated*	4.02	4.62	4.11

*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 4.02 differs from the reported value 3.3 by more than 10 %

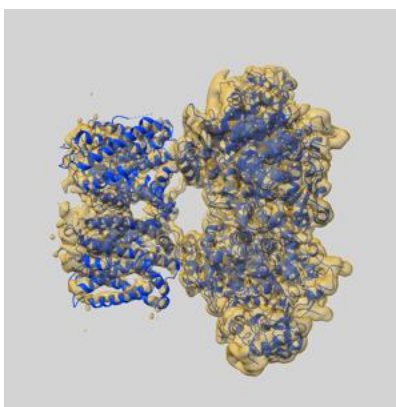
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-40045 and PDB model 8GHG. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

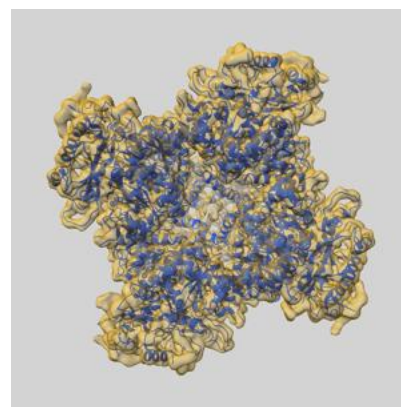
9.1 Map-model overlay [i](#)



X



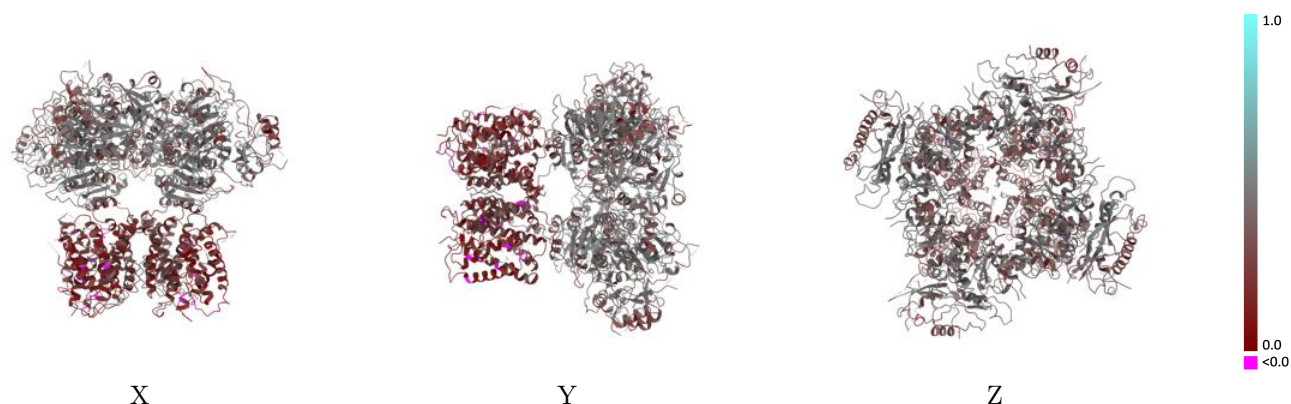
Y



Z

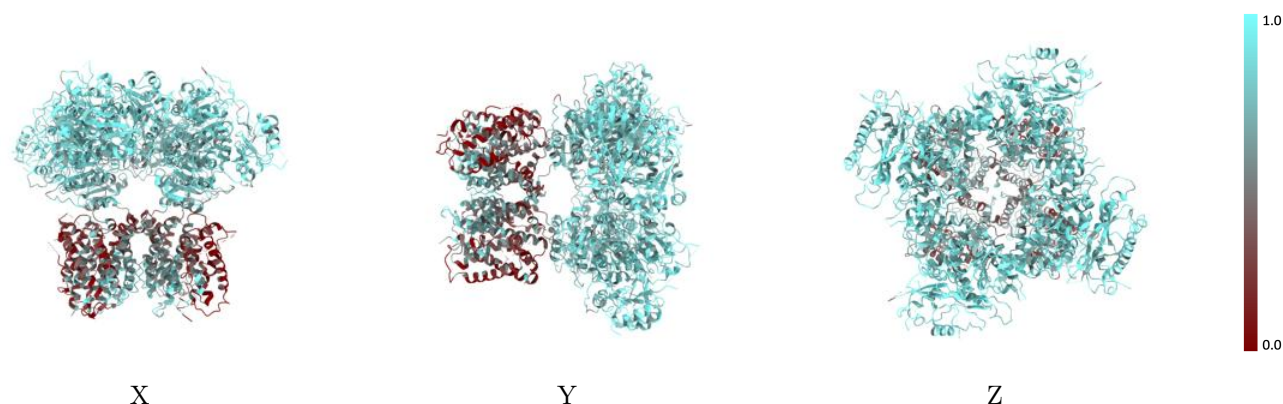
The images above show the 3D surface view of the map at the recommended contour level 0.28 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



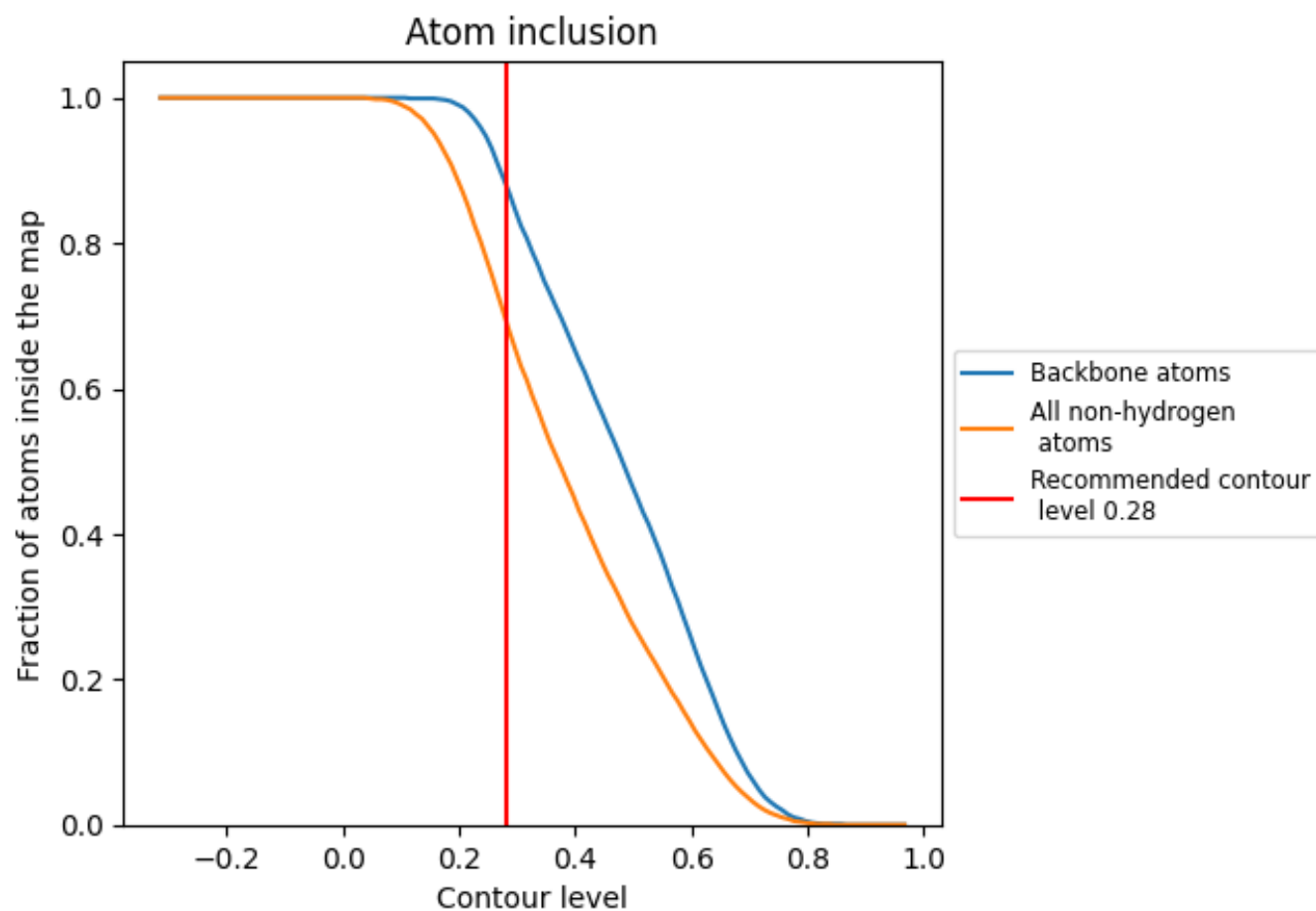
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.28).

9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 70% 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 (0.28) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6960	0.3570
A	0.7050	0.3560
B	0.6980	0.3540
C	0.6900	0.3580
D	0.6890	0.3580

