



wwPDB EM Validation Summary Report ⓘ

Feb 22, 2025 – 02:34 PM EST

PDB ID : 8VLP
EMDB ID : EMD-43341
Title : Composite structure of human FASN with NADPH in State 3
Authors : Schultz, K.; Marmorstein, R.
Deposited on : 2024-01-11
Resolution : 3.20 Å (reported)
Based on initial model : 3HHD

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev117
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

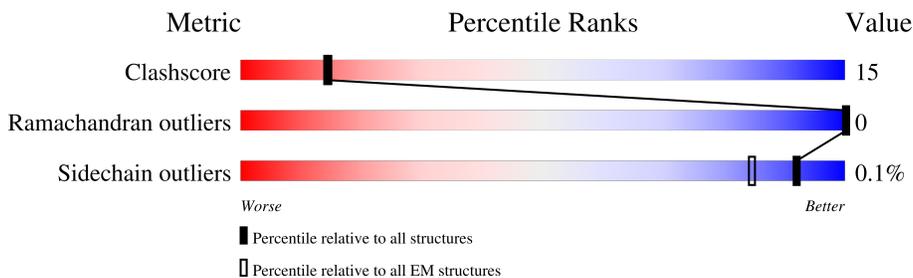
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	2553	
1	B	2553	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 50709 atoms, of which 18827 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 Fatty acid synthase.

Mol	Chain	Residues	Atoms					AltConf	Trace	
			Total	C	H	N	O			S
1	A	2068	Total	C	H	N	O	S	0	0
			25176	10041	9343	2785	2934	73		
1	B	2071	Total	C	H	N	O	S	0	0
			25237	10054	9380	2789	2941	73		

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-31	MET	-	expression tag	UNP P49327
A	-30	SER	-	expression tag	UNP P49327
A	-29	TYR	-	expression tag	UNP P49327
A	-28	TYR	-	expression tag	UNP P49327
A	-27	ASP	-	expression tag	UNP P49327
A	-26	TYR	-	expression tag	UNP P49327
A	-25	LYS	-	expression tag	UNP P49327
A	-24	ASP	-	expression tag	UNP P49327
A	-23	ASP	-	expression tag	UNP P49327
A	-22	ASP	-	expression tag	UNP P49327
A	-21	ASP	-	expression tag	UNP P49327
A	-20	LYS	-	expression tag	UNP P49327
A	-19	ASP	-	expression tag	UNP P49327
A	-18	TYR	-	expression tag	UNP P49327
A	-17	ASP	-	expression tag	UNP P49327
A	-16	ILE	-	expression tag	UNP P49327
A	-15	PRO	-	expression tag	UNP P49327
A	-14	THR	-	expression tag	UNP P49327
A	-13	THR	-	expression tag	UNP P49327
A	-12	GLU	-	expression tag	UNP P49327
A	-11	ASN	-	expression tag	UNP P49327
A	-10	LEU	-	expression tag	UNP P49327
A	-9	TYR	-	expression tag	UNP P49327
A	-8	PHE	-	expression tag	UNP P49327
A	-7	GLN	-	expression tag	UNP P49327
A	-6	GLY	-	expression tag	UNP P49327

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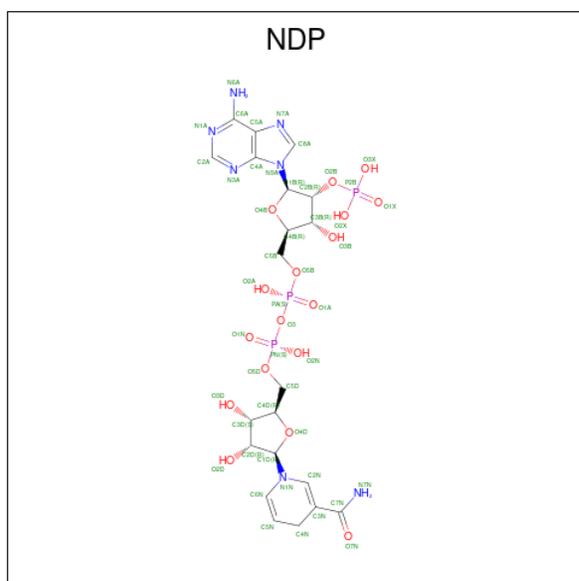
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP P49327
A	-4	MET	-	expression tag	UNP P49327
A	-3	GLY	-	expression tag	UNP P49327
A	-2	SER	-	expression tag	UNP P49327
A	-1	GLY	-	expression tag	UNP P49327
A	0	ILE	-	expression tag	UNP P49327
A	1	PRO	-	expression tag	UNP P49327
A	1151	THR	LYS	conflict	UNP P49327
A	2512	LEU	-	expression tag	UNP P49327
A	2513	GLU	-	expression tag	UNP P49327
A	2514	HIS	-	expression tag	UNP P49327
A	2515	HIS	-	expression tag	UNP P49327
A	2516	HIS	-	expression tag	UNP P49327
A	2517	HIS	-	expression tag	UNP P49327
A	2518	HIS	-	expression tag	UNP P49327
A	2519	HIS	-	expression tag	UNP P49327
A	2520	HIS	-	expression tag	UNP P49327
A	2521	HIS	-	expression tag	UNP P49327
B	-31	MET	-	expression tag	UNP P49327
B	-30	SER	-	expression tag	UNP P49327
B	-29	TYR	-	expression tag	UNP P49327
B	-28	TYR	-	expression tag	UNP P49327
B	-27	ASP	-	expression tag	UNP P49327
B	-26	TYR	-	expression tag	UNP P49327
B	-25	LYS	-	expression tag	UNP P49327
B	-24	ASP	-	expression tag	UNP P49327
B	-23	ASP	-	expression tag	UNP P49327
B	-22	ASP	-	expression tag	UNP P49327
B	-21	ASP	-	expression tag	UNP P49327
B	-20	LYS	-	expression tag	UNP P49327
B	-19	ASP	-	expression tag	UNP P49327
B	-18	TYR	-	expression tag	UNP P49327
B	-17	ASP	-	expression tag	UNP P49327
B	-16	ILE	-	expression tag	UNP P49327
B	-15	PRO	-	expression tag	UNP P49327
B	-14	THR	-	expression tag	UNP P49327
B	-13	THR	-	expression tag	UNP P49327
B	-12	GLU	-	expression tag	UNP P49327
B	-11	ASN	-	expression tag	UNP P49327
B	-10	LEU	-	expression tag	UNP P49327
B	-9	TYR	-	expression tag	UNP P49327
B	-8	PHE	-	expression tag	UNP P49327

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	GLN	-	expression tag	UNP P49327
B	-6	GLY	-	expression tag	UNP P49327
B	-5	ALA	-	expression tag	UNP P49327
B	-4	MET	-	expression tag	UNP P49327
B	-3	GLY	-	expression tag	UNP P49327
B	-2	SER	-	expression tag	UNP P49327
B	-1	GLY	-	expression tag	UNP P49327
B	0	ILE	-	expression tag	UNP P49327
B	1	PRO	-	expression tag	UNP P49327
B	1151	THR	LYS	conflict	UNP P49327
B	2512	LEU	-	expression tag	UNP P49327
B	2513	GLU	-	expression tag	UNP P49327
B	2514	HIS	-	expression tag	UNP P49327
B	2515	HIS	-	expression tag	UNP P49327
B	2516	HIS	-	expression tag	UNP P49327
B	2517	HIS	-	expression tag	UNP P49327
B	2518	HIS	-	expression tag	UNP P49327
B	2519	HIS	-	expression tag	UNP P49327
B	2520	HIS	-	expression tag	UNP P49327
B	2521	HIS	-	expression tag	UNP P49327

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf	
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

LEU	V1680	E1435	V1245	VAL	PRO	L759	P892	E629	V550	F450	M329	V231	M139
VAL	Q1714	R1439	L1246	THR	SER	E760	P693	C630	H651	V460	G330	L252	N142
GLU	E1750	A1445	G1250	GLN	A859	A762	L695	K631	F553	P461	H331	T234	R143
THR	H1763	I1446	LEU	GLY	T879	P763	Q696	P635	S554	A464	P332	K235	L144
ASN	H1788	I1450	MET	LEU	R901	A765	L698	P636	V555	R468	E333	L238	S145
ASP	D1773	T1450	VAL	VAL	V912	L766	V701	G637	I559	R469	P334	L238	F146
THR	S1451	T1450	VAL	VAL	V913	Q768	I702	V639	Q560	G469	A335	V242	A156
ILE	G1452	G1452	PRO	PRO	A769	A769	R703	P640	Q560	L338	G337	N248	L157
VAL	V1453	V1453	GLY	LEU	L771	V770	E704	A641	I564	A249	A339	A249	T159
S2081	V1454	V1454	ASP	ASP	K772	K772	K706	C642	L567	L341	L341	G250	C161
P2085	V1457	V1457	GLY	GLY	R773	G774	R707	H644	S668	A340	A340	T251	S162
L2097	R1468	R1468	ALA	ALA	G774	G774	R708	S645	C569	K343	K343	N252	S163
E2113	C1471	C1471	ILE	ILE	K776	K776	R711	K646	M570	F494	F494	K257	S164
ALA	L1474	L1474	PRO	PRO	P777	P777	T648	D847	T648	I495	I495	F263	L165
ALA	D1487	D1487	ARG	ARG	S778	S778	W712	T649	P574	M499	M499	F263	M166
ALA	A1282	A1282	ASP	ASP	I781	I781	L713	V649	D575	G500	G500	D257	A167
ALA	A1283	A1283	ASP	ASP	P783	P783	S714	T650	G576	T501	T501	Q271	A182
TYR	G1295	G1295	ASP	ASP	L784	L784	I717	S852	I577	Q502	Q502	L272	I188
ARG	P1299	P1299	ASP	ASP	R790	R790	P718	G853	S881	M503	M503	L272	M189
ARG	A1300	A1300	ASP	ASP	D791	D791	E719	P654	L82	M504	M504	R274	I189
ARG	L1312	L1312	ASP	ASP	E794	E794	A720	Q655	L82	G505	G505	L273	I190
ASP	C1315	C1315	ASP	ASP	L803	L803	A720	Q655	L82	G505	G505	L273	L191
ASP	M1316	M1316	ASP	ASP	H804	H804	A720	Q655	L82	G505	G505	L273	L191
ASP	V1319	V1319	ASP	ASP	L805	L805	A720	Q655	L82	G505	G505	L273	L191
ASP	S1327	S1327	ASP	ASP	A810	A810	A720	Q655	L82	G505	G505	L273	L191
ASP	M1331	M1331	ASP	ASP	N811	N811	A720	Q655	L82	G505	G505	L273	L191
ASP	M1332	M1332	ASP	ASP	P812	P812	A720	Q655	L82	G505	G505	L273	L191
ASP	L1348	L1348	ASP	ASP	N813	N813	A720	Q655	L82	G505	G505	L273	L191
ASP	R1349	R1349	ASP	ASP	A814	A814	A720	Q655	L82	G505	G505	L273	L191
ASP	I1356	I1356	ASP	ASP	P822	P822	A720	Q655	L82	G505	G505	L273	L191
ASP	E1364	E1364	ASP	ASP	A823	A823	A720	Q655	L82	G505	G505	L273	L191
ASP	P1365	P1365	ASP	ASP	P824	P824	A720	Q655	L82	G505	G505	L273	L191
ASP	Q1366	Q1366	ASP	ASP	L833	L833	A720	Q655	L82	G505	G505	L273	L191
ASP	Y1367	Y1367	ASP	ASP	W836	W836	A720	Q655	L82	G505	G505	L273	L191
ASP	G1368	G1368	ASP	ASP	D837	D837	A720	Q655	L82	G505	G505	L273	L191
ASP	Q1369	Q1369	ASP	ASP	H838	H838	A720	Q655	L82	G505	G505	L273	L191
ASP	G1370	G1370	ASP	ASP	W842	W842	A720	Q655	L82	G505	G505	L273	L191
ASP	I1371	I1371	ASP	ASP	E848	E848	A720	Q655	L82	G505	G505	L273	L191
ASP	L1372	L1372	ASP	ASP	N852	N852	A720	Q655	L82	G505	G505	L273	L191
ASP	S1373	S1373	ASP	ASP	GLY	GLY	A720	Q655	L82	G505	G505	L273	L191
ASP	Q1374	Q1374	ASP	ASP	SER	SER	A720	Q655	L82	G505	G505	L273	L191
ASP	L1391	L1391	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	K1392	K1392	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	V1417	V1417	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	K1429	K1429	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	V1650	V1650	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	V1651	V1651	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	V1652	V1652	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	S1653	S1653	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	T1654	T1654	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	G1867	G1867	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	A1868	A1868	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	K1869	K1869	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	I1876	I1876	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	T1879	T1879	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	R1907	R1907	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	Q1928	Q1928	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	R1931	R1931	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	E1981	E1981	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	Y1996	Y1996	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	S2020	S2020	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	S2021	S2021	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	V2022	V2022	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	R2026	R2026	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	N2033	N2033	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	Y2034	Y2034	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	E2042	E2042	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	Q2059	Q2059	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	W2060	W2060	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	V2066	V2066	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	GLY	GLY	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	ILE	ILE	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	L2128	L2128	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	V1242	V1242	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	L1177	L1177	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	L1178	L1178	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	R1187	R1187	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	L1188	L1188	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	Q1189	Q1189	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	L1190	L1190	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	N1191	N1191	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	G1192	G1192	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	N1193	N1193	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	L1194	L1194	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	Q1195	Q1195	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	L1196	L1196	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	E1197	E1197	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	A1199	A1199	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	Q1200	Q1200	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	V1201	V1201	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	L1202	L1202	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	A1203	A1203	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	Q1204	Q1204	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	E1205	E1205	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	R1206	R1206	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	P1207	P1207	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	K1208	K1208	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	L1209	L1209	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	P1210	P1210	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	P1213	P1213	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	L1214	L1214	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	L1215	L1215	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	S1216	S1216	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	G1217	G1217	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	L1228	L1228	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	V1242	V1242	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	E1594	E1594	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	Q1595	Q1595	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	D1596	D1596	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	E1602	E1602	ASP	ASP	THR	THR	A720	Q655	L82	G505	G505	L273	L191
ASP	R1606	R											

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	131766	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	52.4	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	81000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.757	Depositor
Minimum map value	-0.203	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.197	Depositor
Map size (\AA)	384.84, 384.84, 384.84	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.069, 1.069, 1.069	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

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	0.27	0/16198	0.47	0/22023
1	B	0.28	0/16222	0.48	0/22055
All	All	0.27	0/32420	0.48	0/44078

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	15833	9343	15809	504	0
1	B	15857	9380	15826	477	0
2	A	96	52	52	4	0
2	B	96	52	52	0	0
All	All	31882	18827	31739	966	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 15.

The worst 5 of 966 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:625:LEU:HD11	1:A:629:GLU:HB2	1.34	1.08
1:B:9:MET:HE1	1:B:342:ALA:HA	1.38	1.04
1:A:628:GLU:HA	1:A:631:LYS:HE2	1.41	1.02
1:A:164:SER:HB2	1:A:338:LEU:HD13	1.46	0.97
1:A:564:ILE:HD13	1:A:590:ALA:HB2	1.53	0.92

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	2060/2553 (81%)	2021 (98%)	39 (2%)	0	100	100
1	B	2063/2553 (81%)	2026 (98%)	37 (2%)	0	100	100
All	All	4123/5106 (81%)	4047 (98%)	76 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1705/2117 (80%)	1703 (100%)	2 (0%)	92	98
1	B	1708/2117 (81%)	1708 (100%)	0	100	100
All	All	3413/4234 (81%)	3411 (100%)	2 (0%)	92	98

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	277	TYR
1	A	1896	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	580	HIS
1	B	142	ASN
1	B	768	GLN
1	B	1331	ASN
1	B	1345	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	NDP	A	2601	-	47,52,52	0.65	0	61,80,80	0.87	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NDP	A	2602	-	47,52,52	0.66	0	61,80,80	0.80	2 (3%)
2	NDP	B	2601	-	47,52,52	0.68	0	61,80,80	0.77	2 (3%)
2	NDP	B	2602	-	47,52,52	0.65	0	61,80,80	0.88	3 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	A	2601	-	-	12/30/77/77	0/5/5/5
2	NDP	A	2602	-	-	8/30/77/77	0/5/5/5
2	NDP	B	2601	-	-	11/30/77/77	0/5/5/5
2	NDP	B	2602	-	-	10/30/77/77	0/5/5/5

There are no bond length outliers.

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2602	NDP	P2B-O2B-C2B	-3.97	112.82	123.43
2	A	2602	NDP	P2B-O2B-C2B	-3.90	113.01	123.43
2	A	2601	NDP	C4B-O4B-C1B	-2.81	107.36	109.92
2	B	2601	NDP	P2B-O2B-C2B	-2.66	116.32	123.43
2	B	2602	NDP	C3N-C2N-N1N	-2.57	119.44	123.20

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

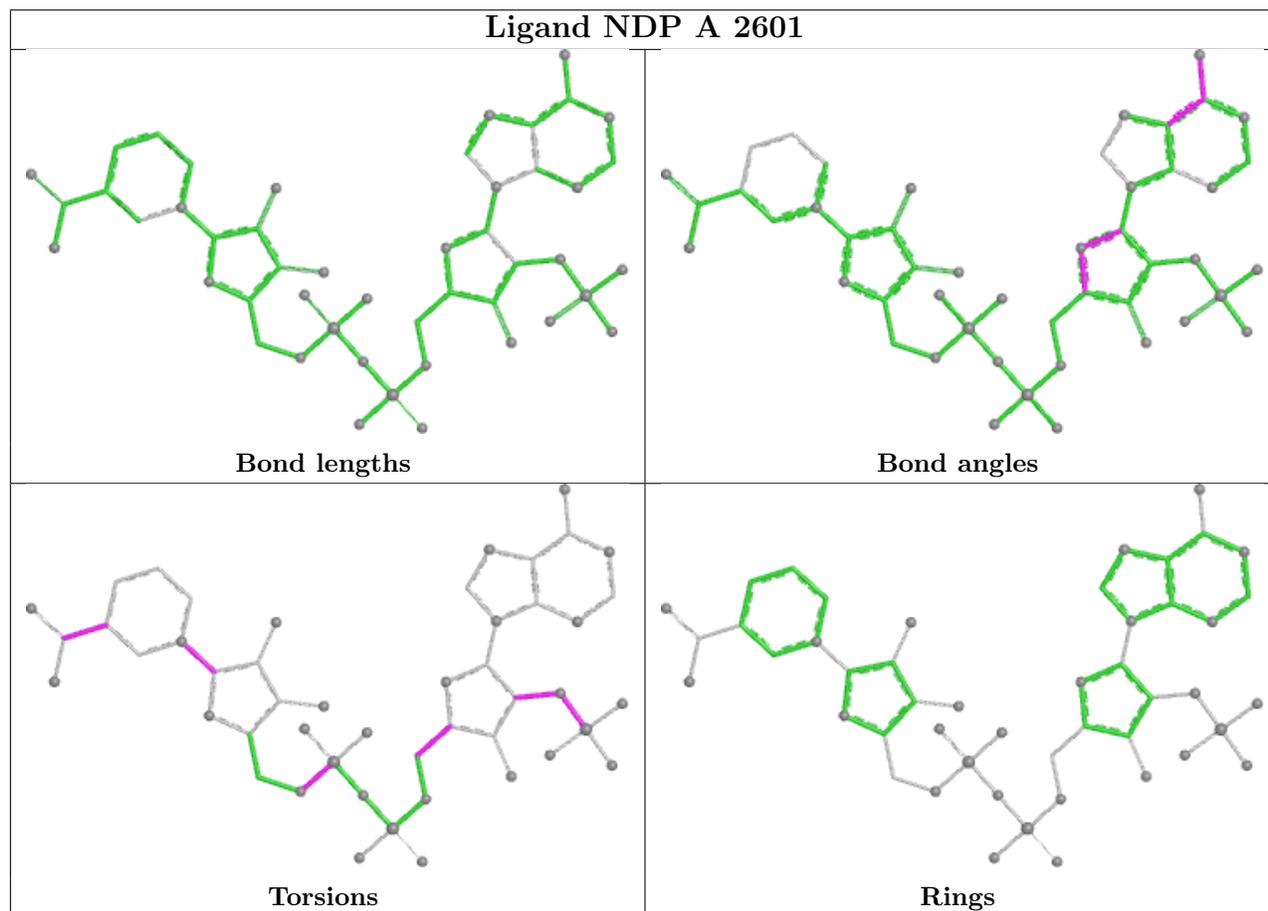
Mol	Chain	Res	Type	Atoms
2	A	2601	NDP	C5D-O5D-PN-O3
2	A	2601	NDP	C5D-O5D-PN-O1N
2	A	2601	NDP	O4D-C1D-N1N-C2N
2	A	2601	NDP	C2N-C3N-C7N-N7N
2	A	2602	NDP	C5B-O5B-PA-O2A

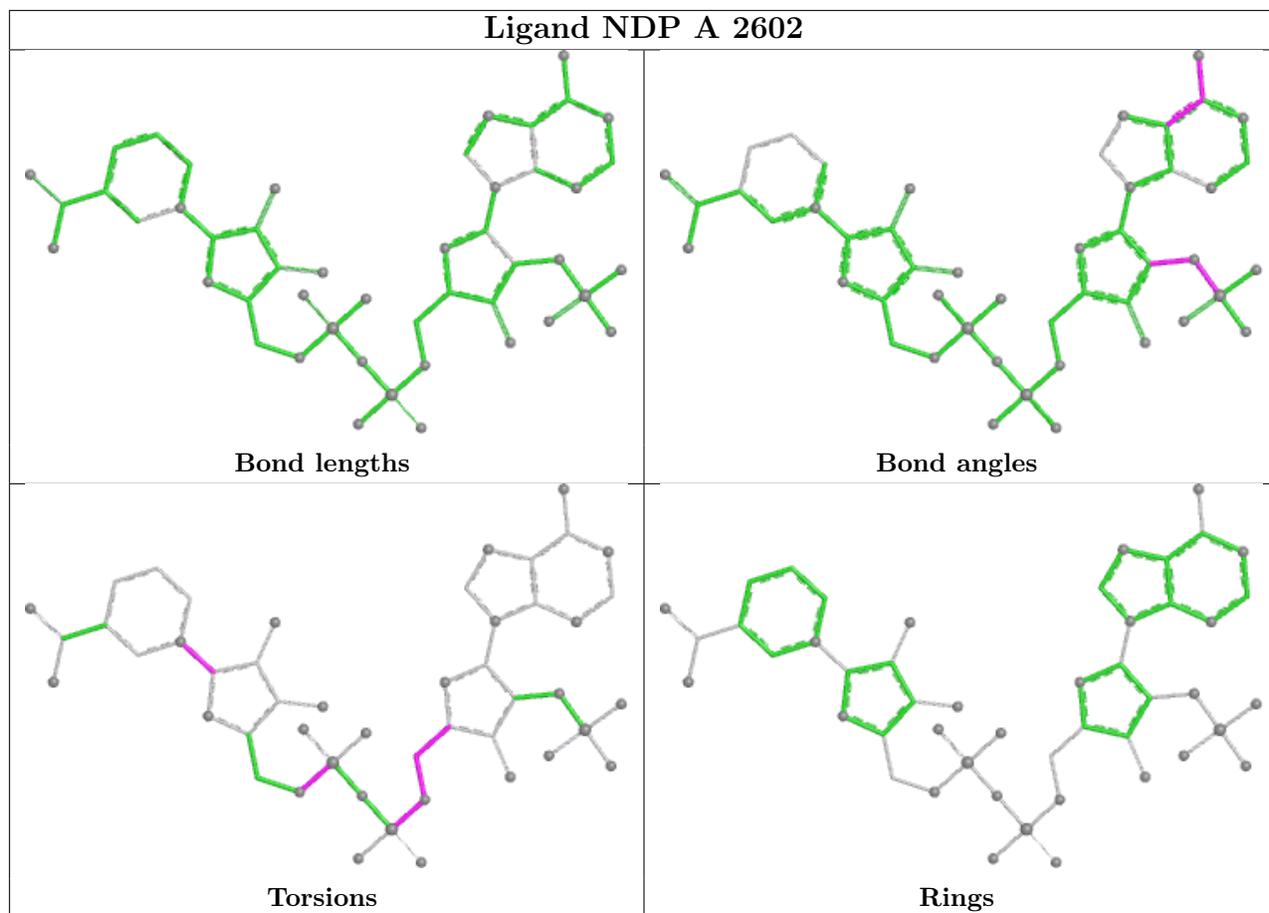
There are no ring outliers.

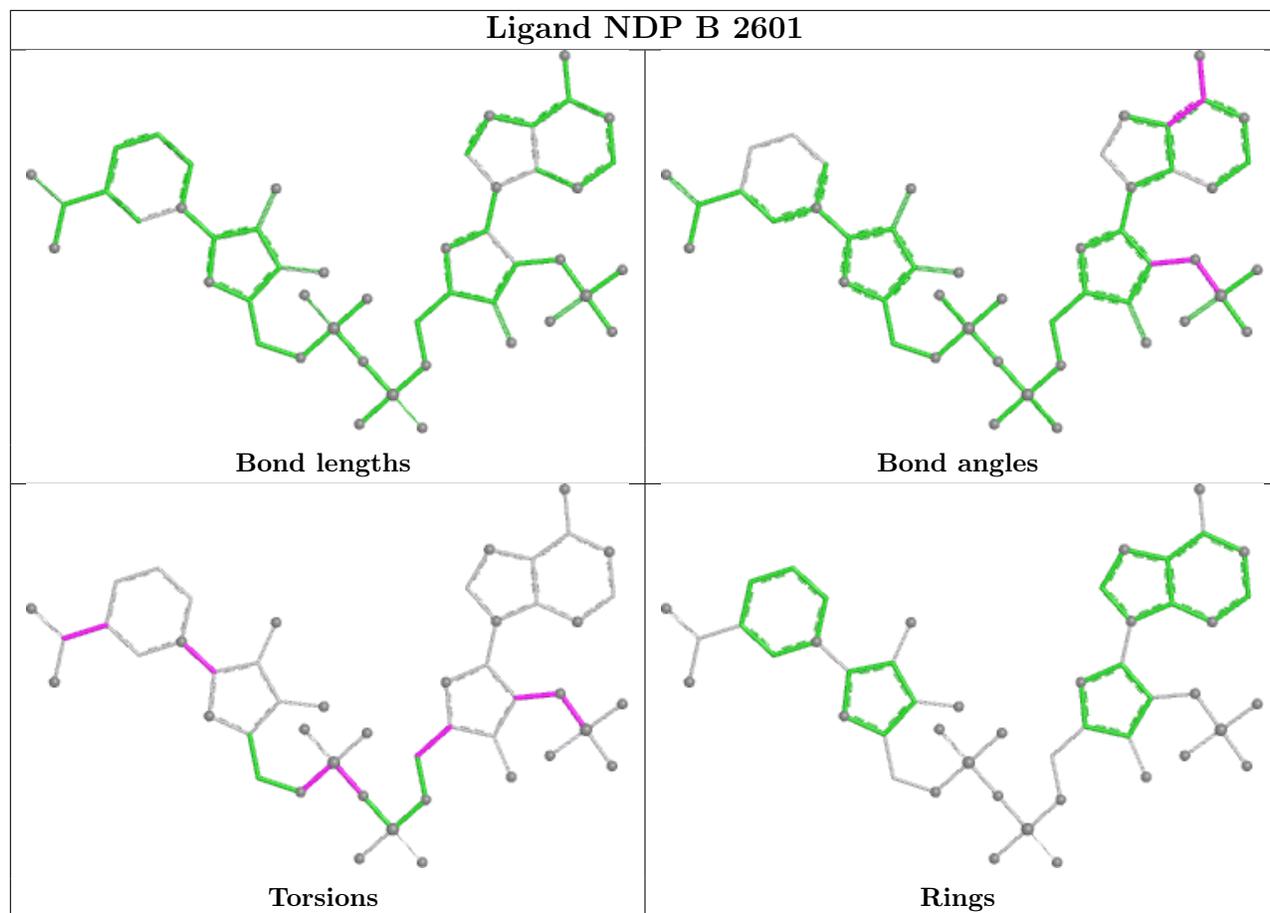
2 monomers are involved in 4 short contacts:

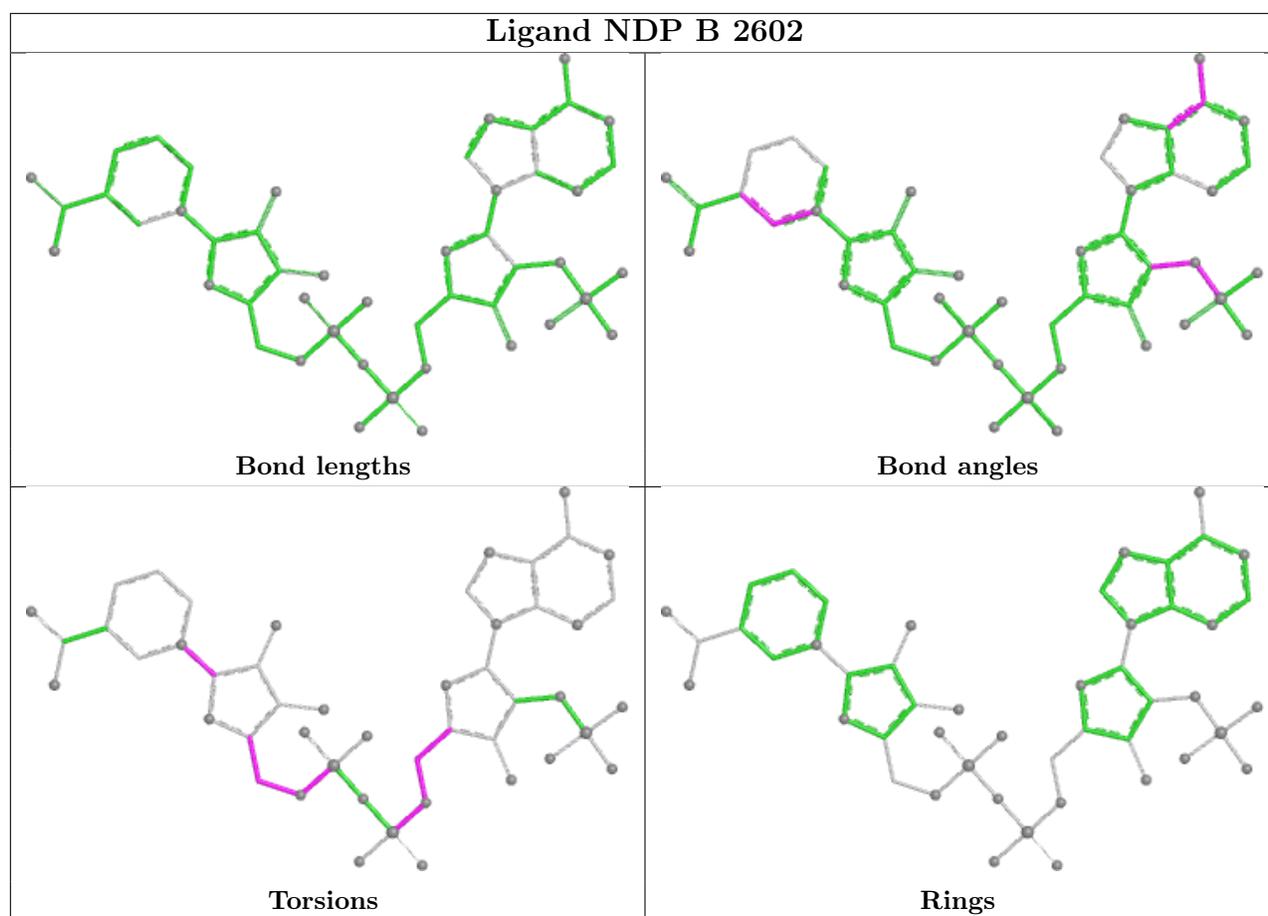
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2601	NDP	1	0
2	A	2602	NDP	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

There are no chain breaks in this entry.

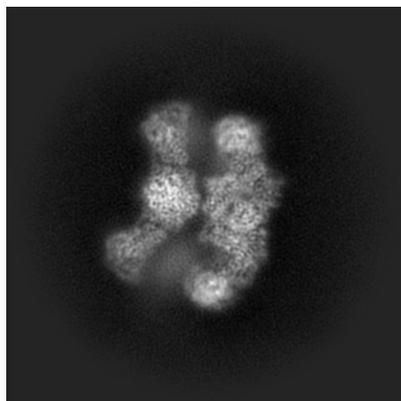
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43341. These allow visual inspection of the internal detail of the map and identification of artifacts.

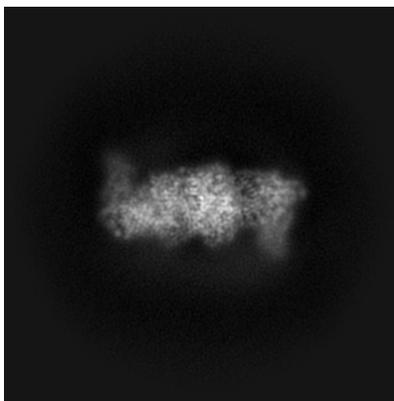
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

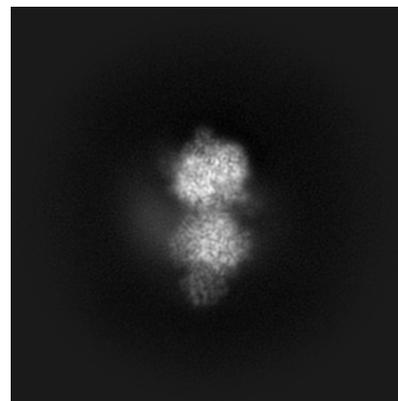
6.1.1 Primary map



X

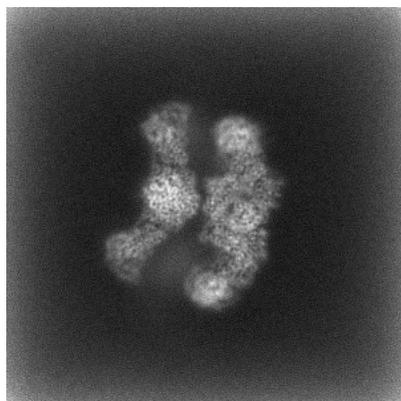


Y

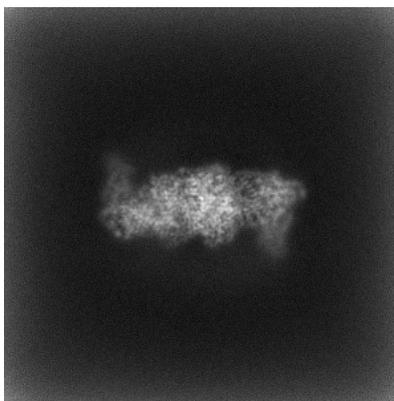


Z

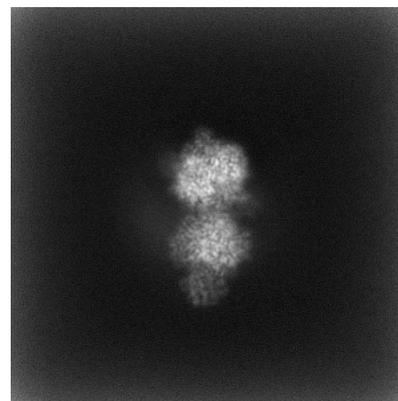
6.1.2 Raw map



X



Y

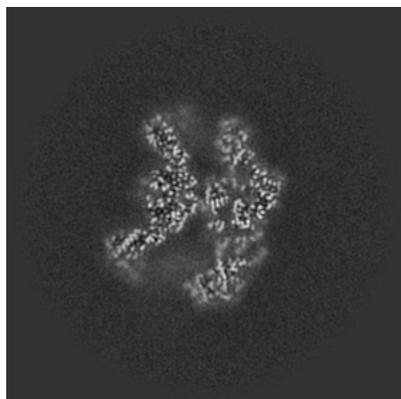


Z

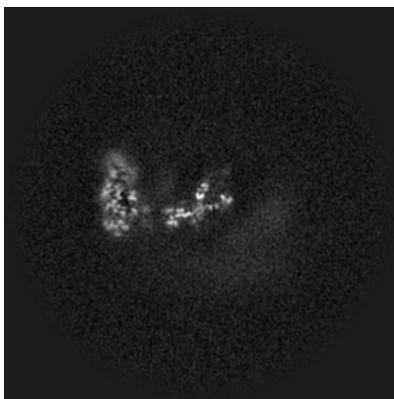
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

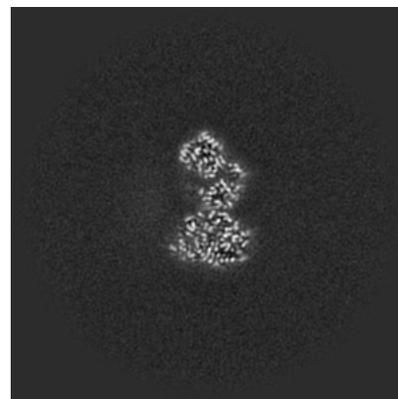
6.2.1 Primary map



X Index: 180

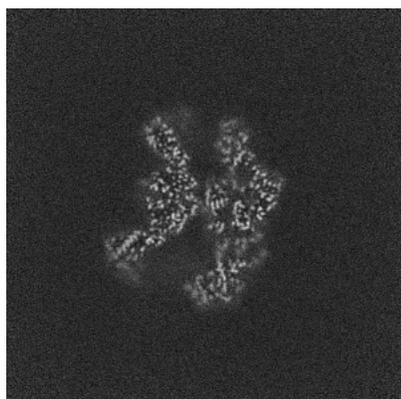


Y Index: 180



Z Index: 180

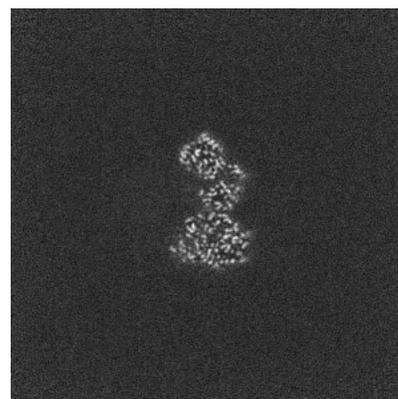
6.2.2 Raw map



X Index: 180



Y Index: 180

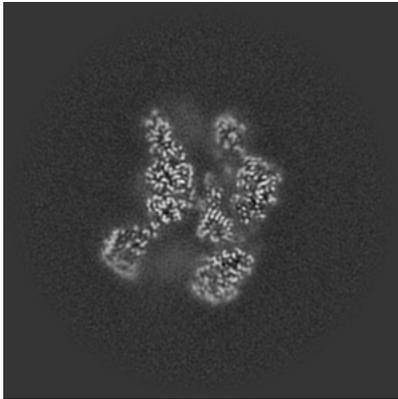


Z Index: 180

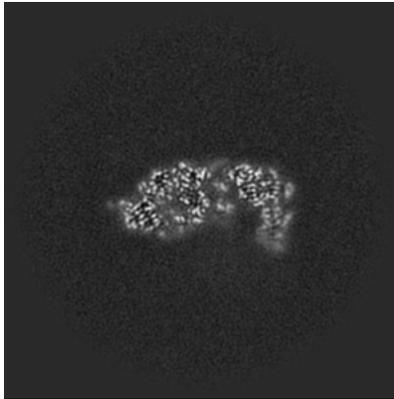
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

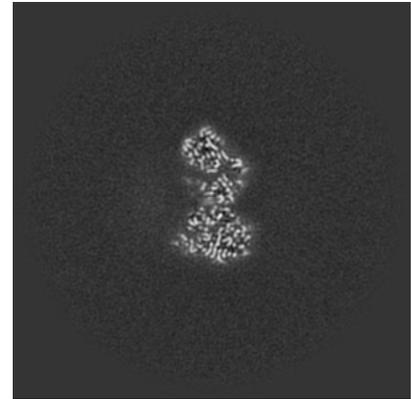
6.3.1 Primary map



X Index: 175

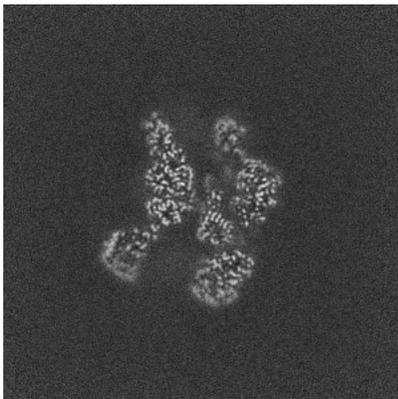


Y Index: 212

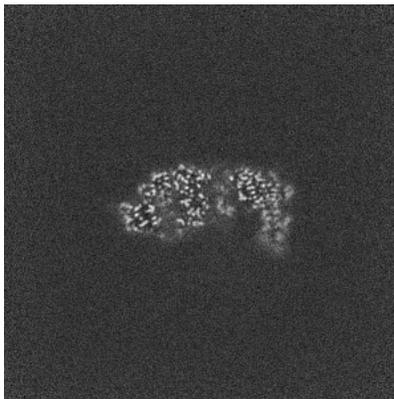


Z Index: 179

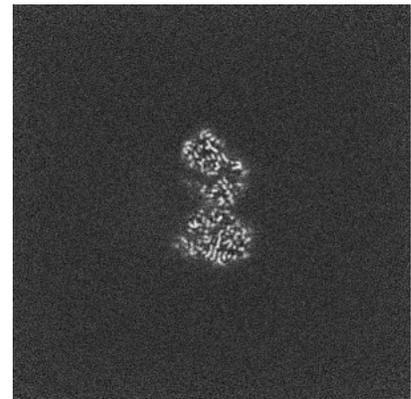
6.3.2 Raw map



X Index: 175



Y Index: 213

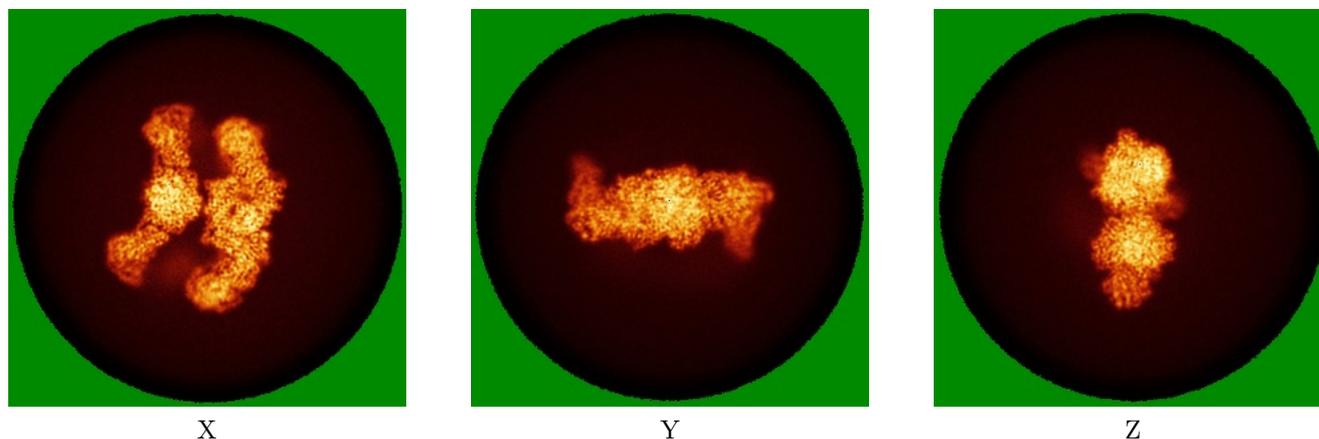


Z Index: 179

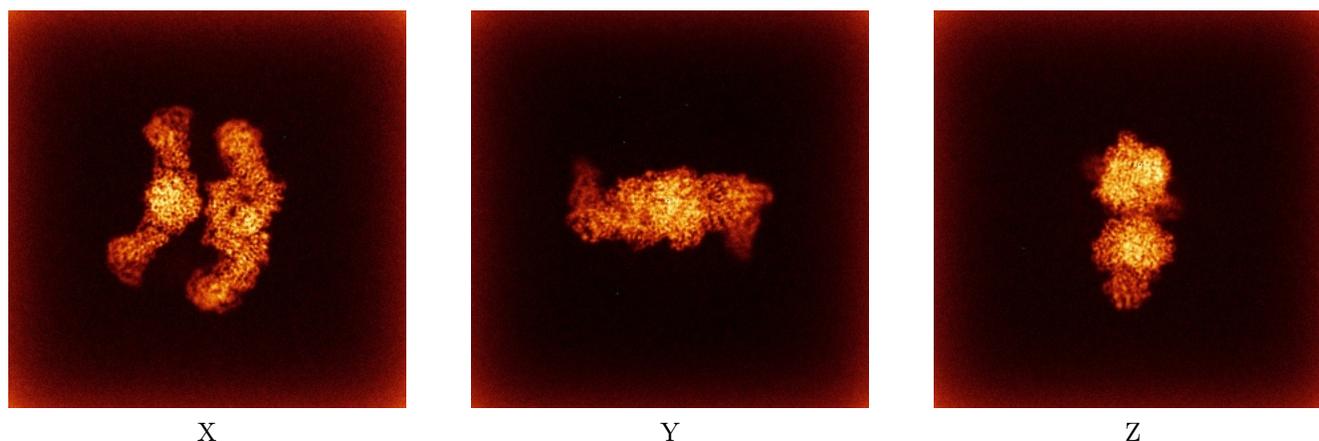
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



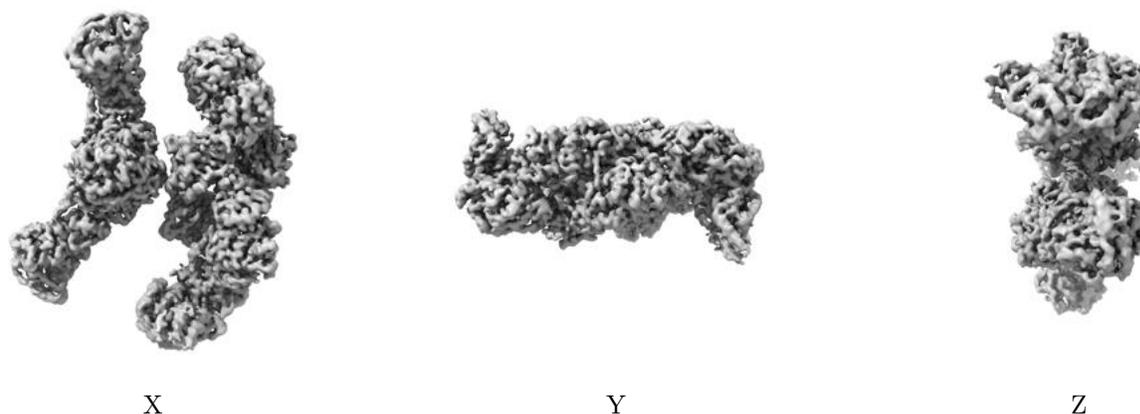
6.4.2 Raw map



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.

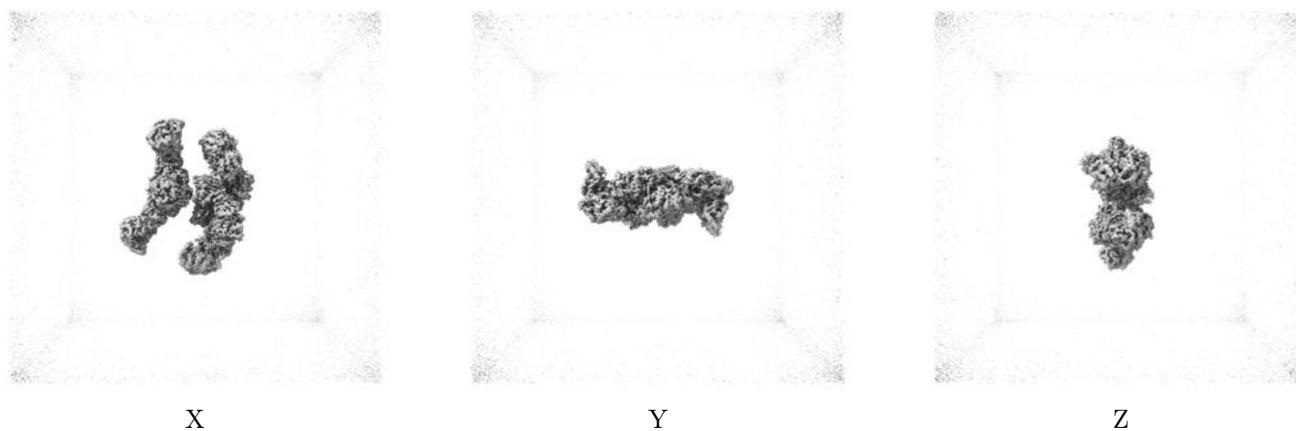
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.197. 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.

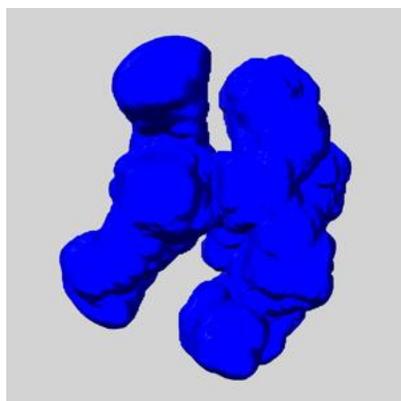
6.6 Mask visualisation [i](#)

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

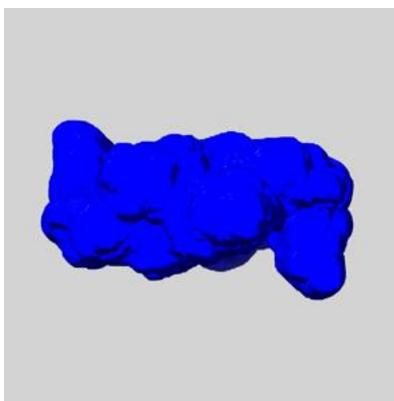
A mask typically either:

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

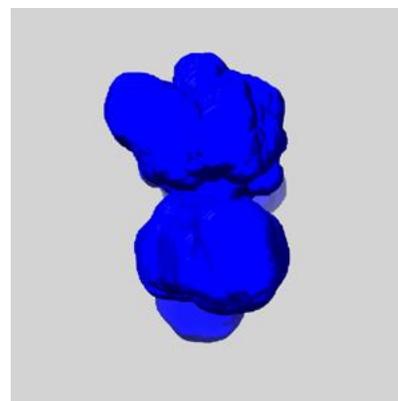
6.6.1 emd_43341_msk_1.map [i](#)



X



Y

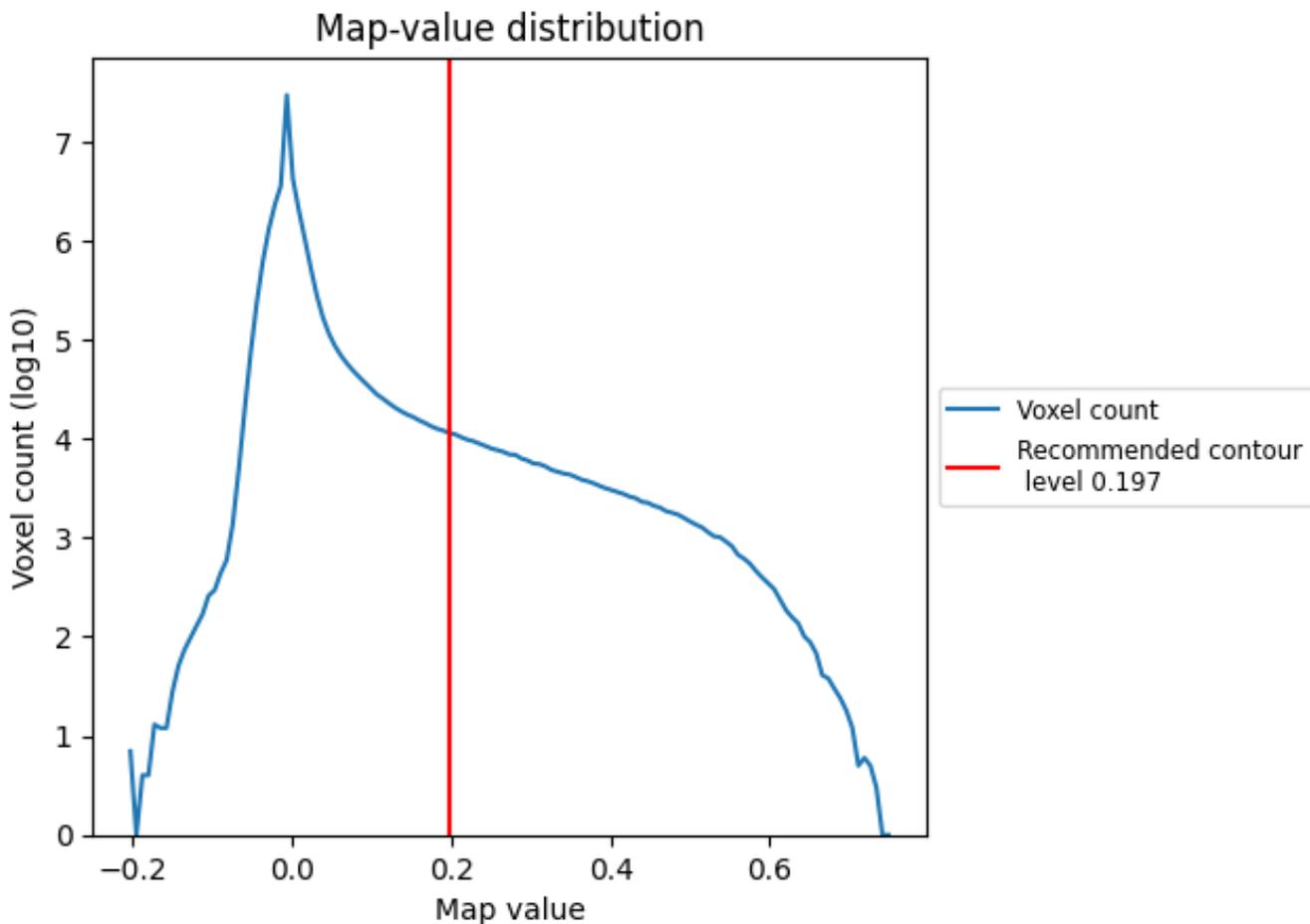


Z

7 Map analysis [i](#)

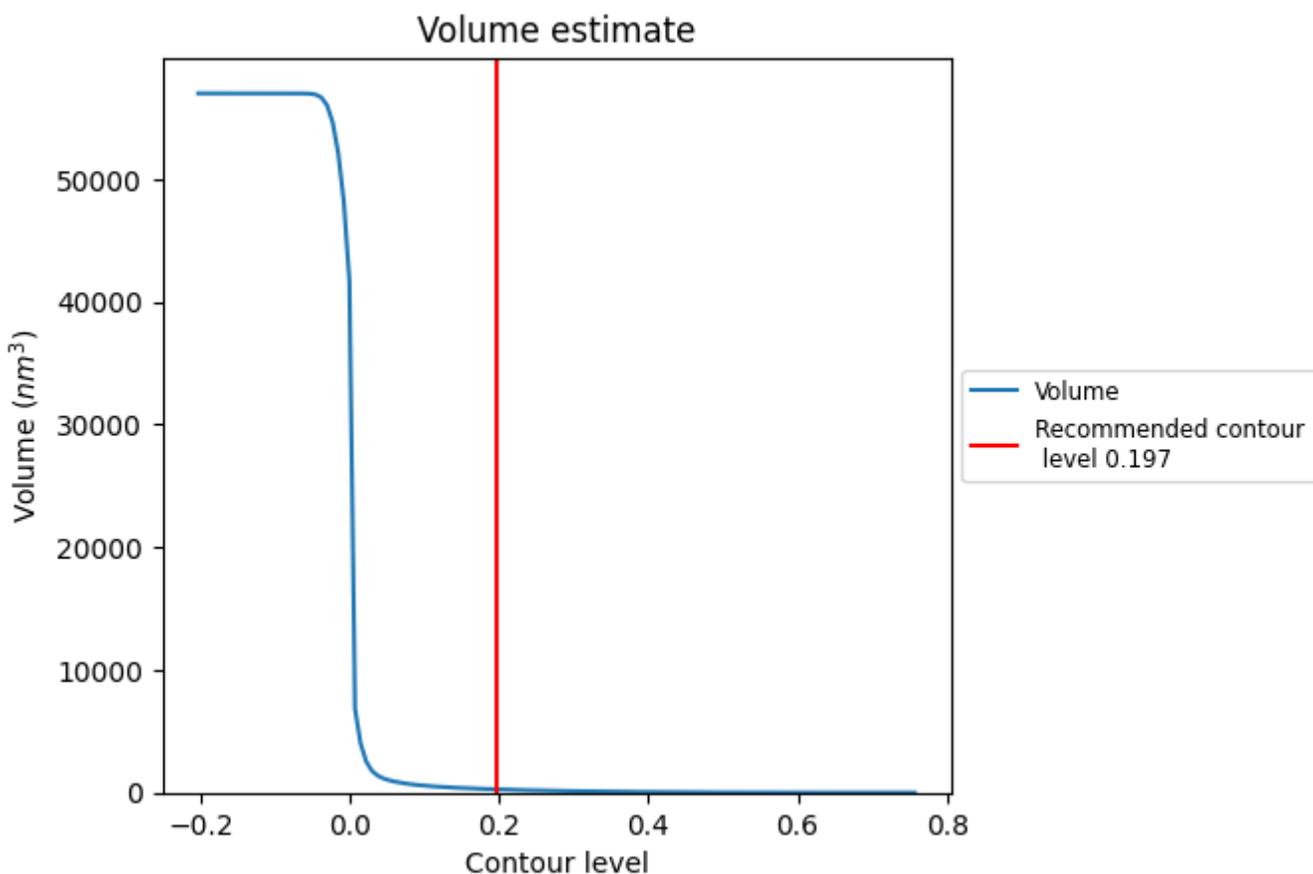
This section contains the results of statistical analysis of the map.

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.

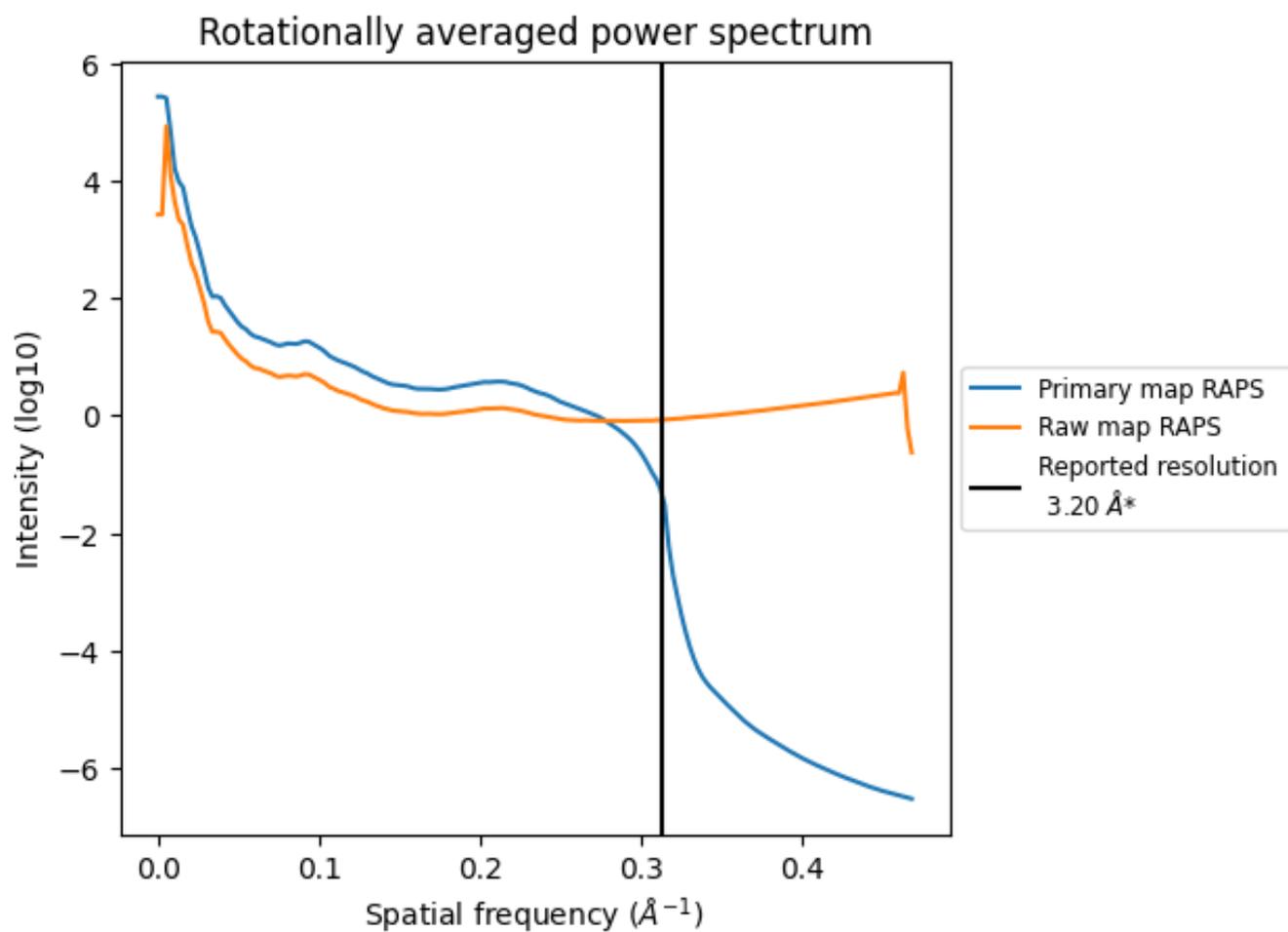
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 267 nm³; this corresponds to an approximate mass of 241 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum [i](#)

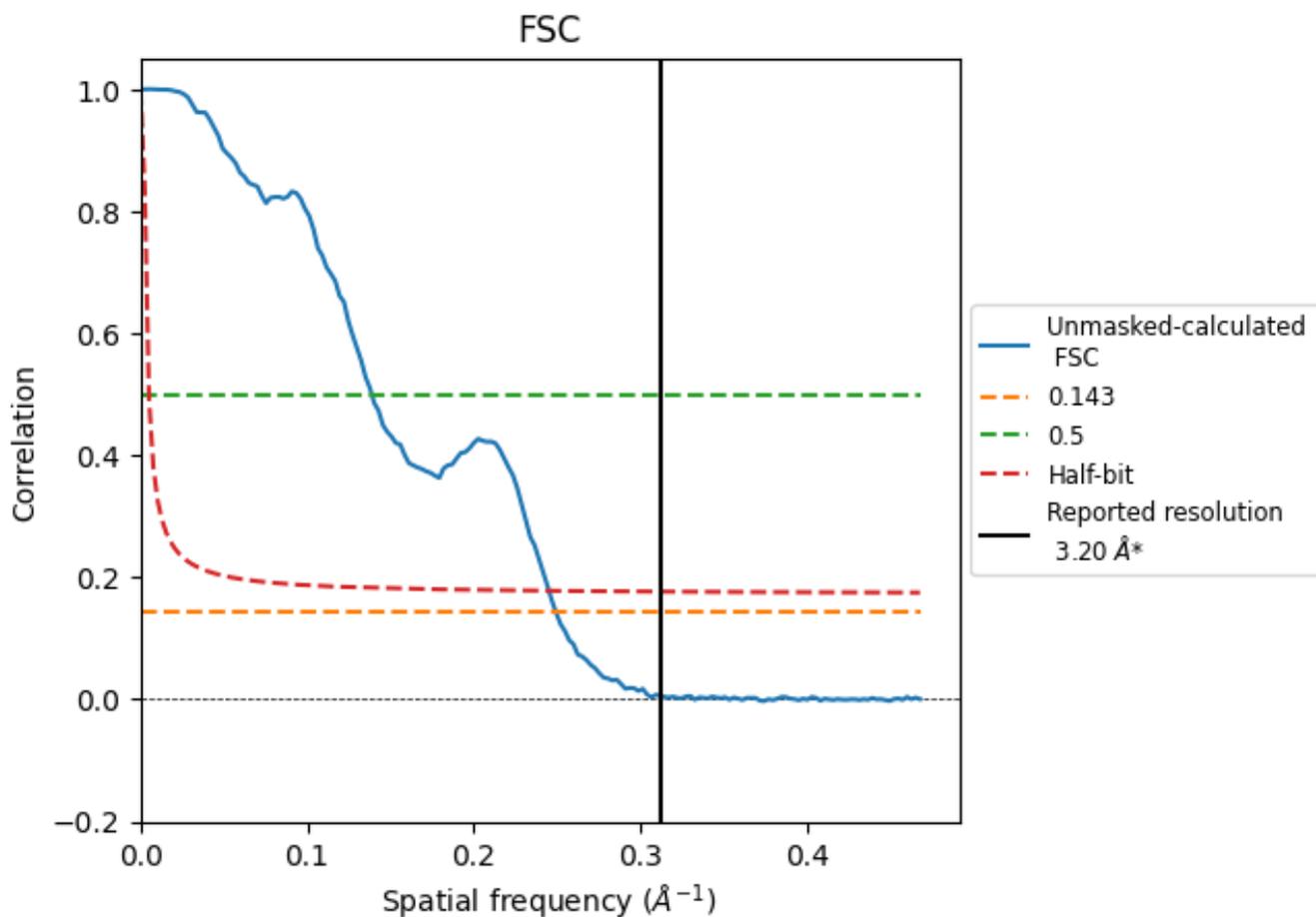


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

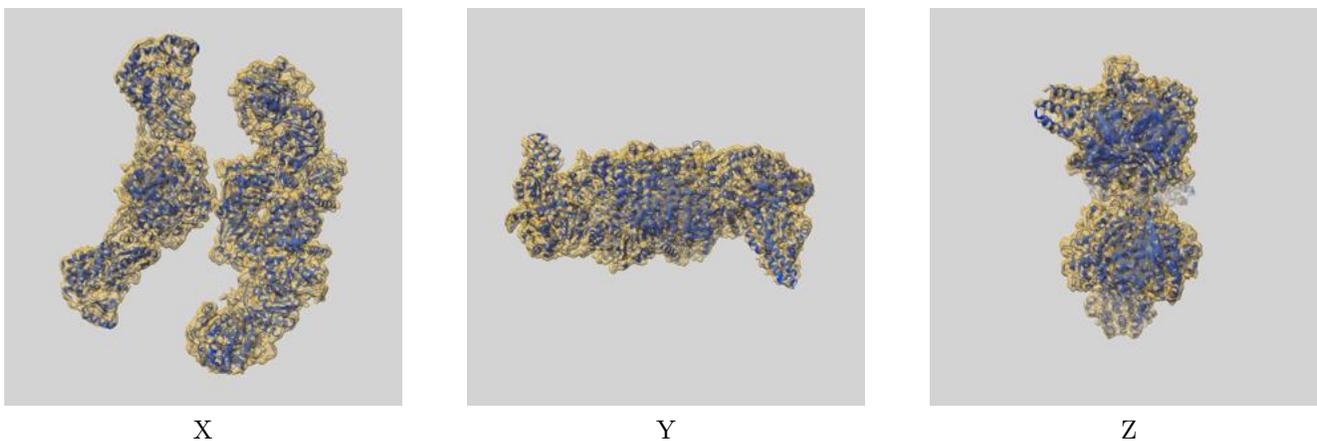
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	7.20	4.08

*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 4.01 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

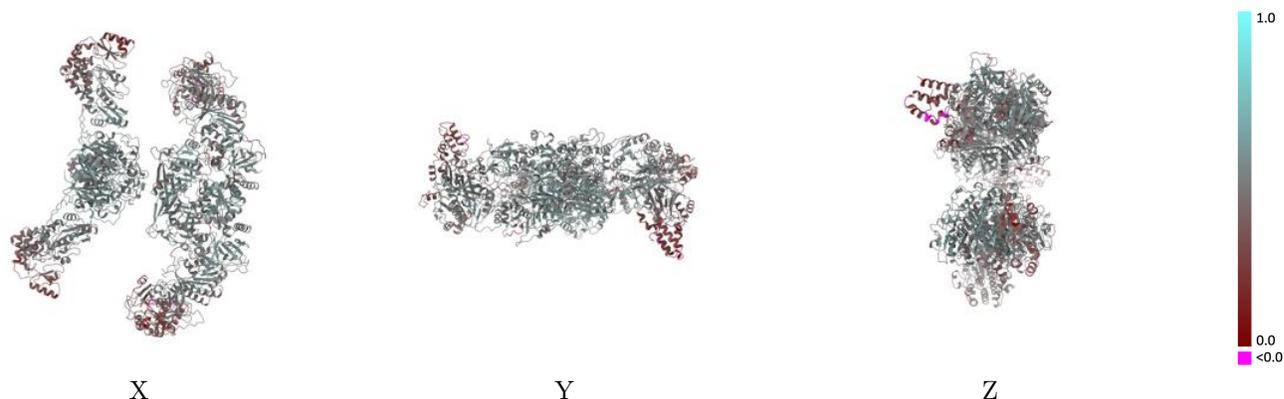
This section contains information regarding the fit between EMDB map EMD-43341 and PDB model 8VLP. Per-residue inclusion information can be found in section 3 on page 7.

9.1 Map-model overlay [i](#)



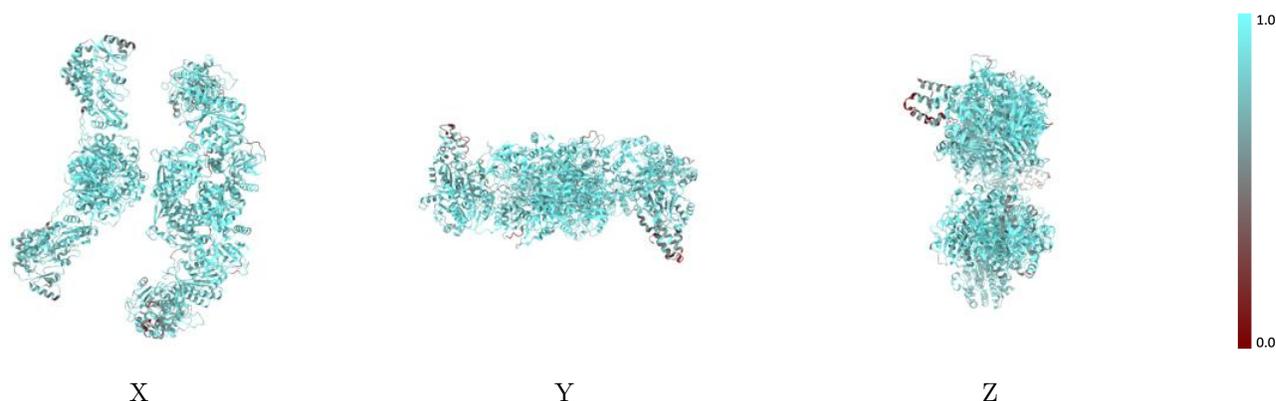
The images above show the 3D surface view of the map at the recommended contour level 0.197 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



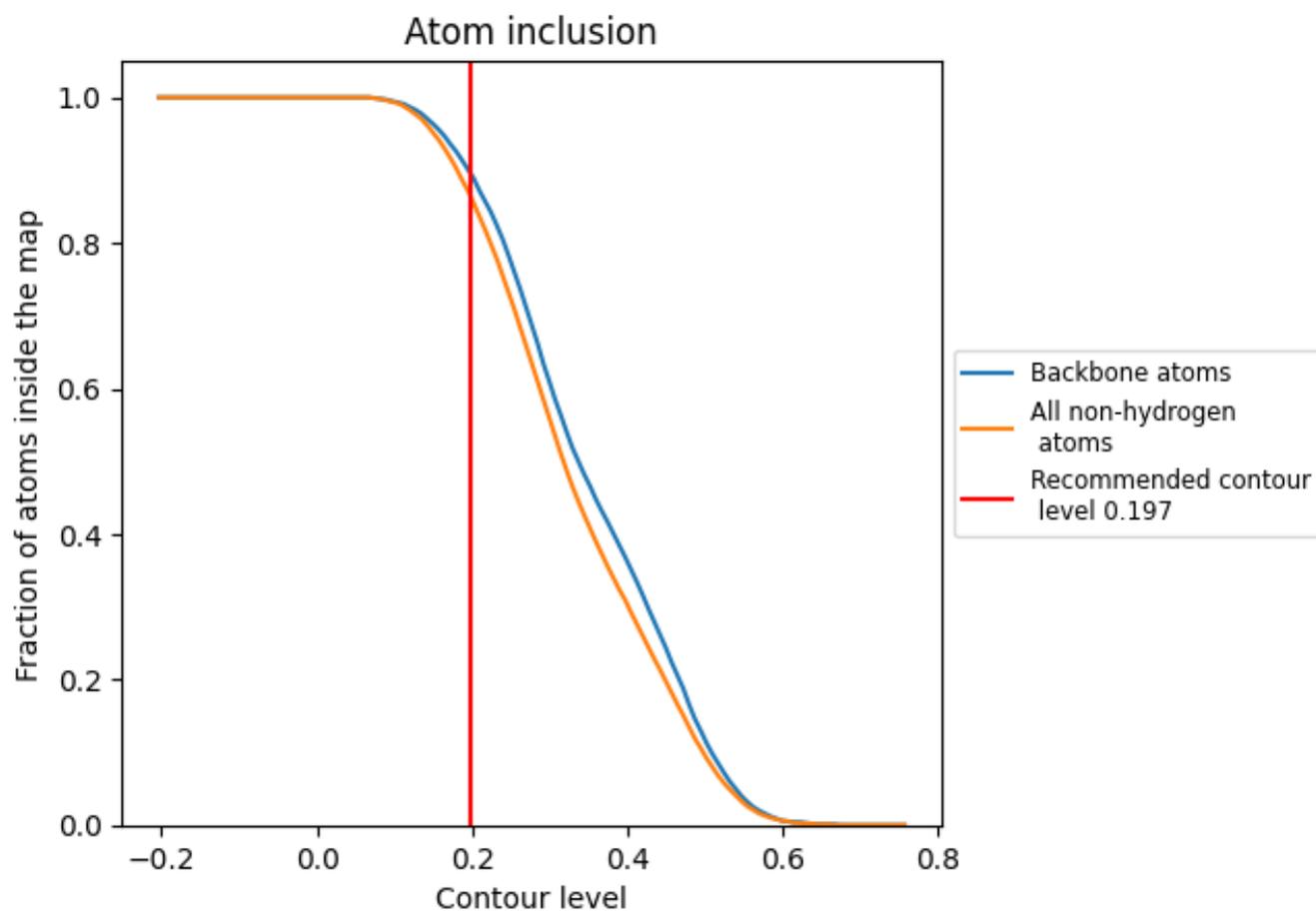
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.197).

9.4 Atom inclusion [i](#)



At the recommended contour level, 90% of all backbone atoms, 87% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary [i](#)

The table lists the average atom inclusion at the recommended contour level (0.197) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8670	 0.4740
A	 0.8690	 0.4750
B	 0.8650	 0.4730

