



## wwPDB EM Validation Summary Report ⓘ

Feb 22, 2025 – 03:27 PM EST

PDB ID : 8VM7  
EMDB ID : EMD-43354  
Title : Composite structure of human FASN with NADPH in State 7  
Authors : Schultz, K.; Marmorstein, R.  
Deposited on : 2024-01-13  
Resolution : 3.30 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](mailto: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

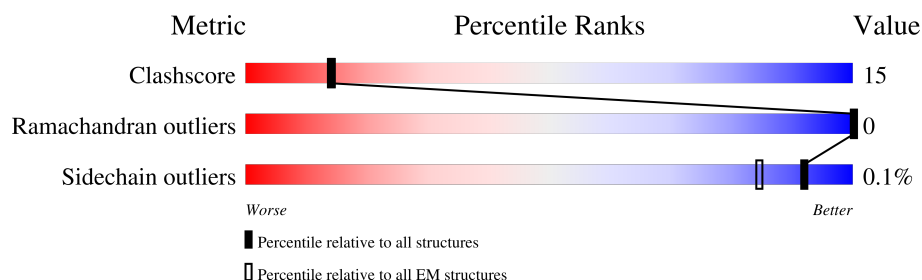
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.30 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)
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  $\geq 3$ , 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	 59% 22% 19%
1	B	2553	 60% 21% 19%

## 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
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

*Continued on next page...*

*Continued from previous page...*

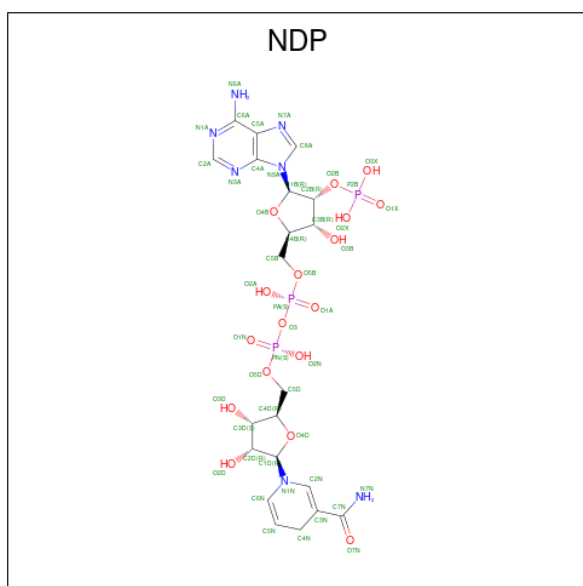
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP P49327
A	-4	MET	-	expression tag	UNP P49327
A	-3	GLY	-	expression tag	UNP P49327
A	-2	SER	-	expression tag	UNP P49327
A	-1	GLY	-	expression tag	UNP P49327
A	0	ILE	-	expression tag	UNP P49327
A	1	PRO	-	expression tag	UNP P49327
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

*Continued on next page...*

Continued from previous page...

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<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>) (labeled as "Ligand of Interest" by depositor).

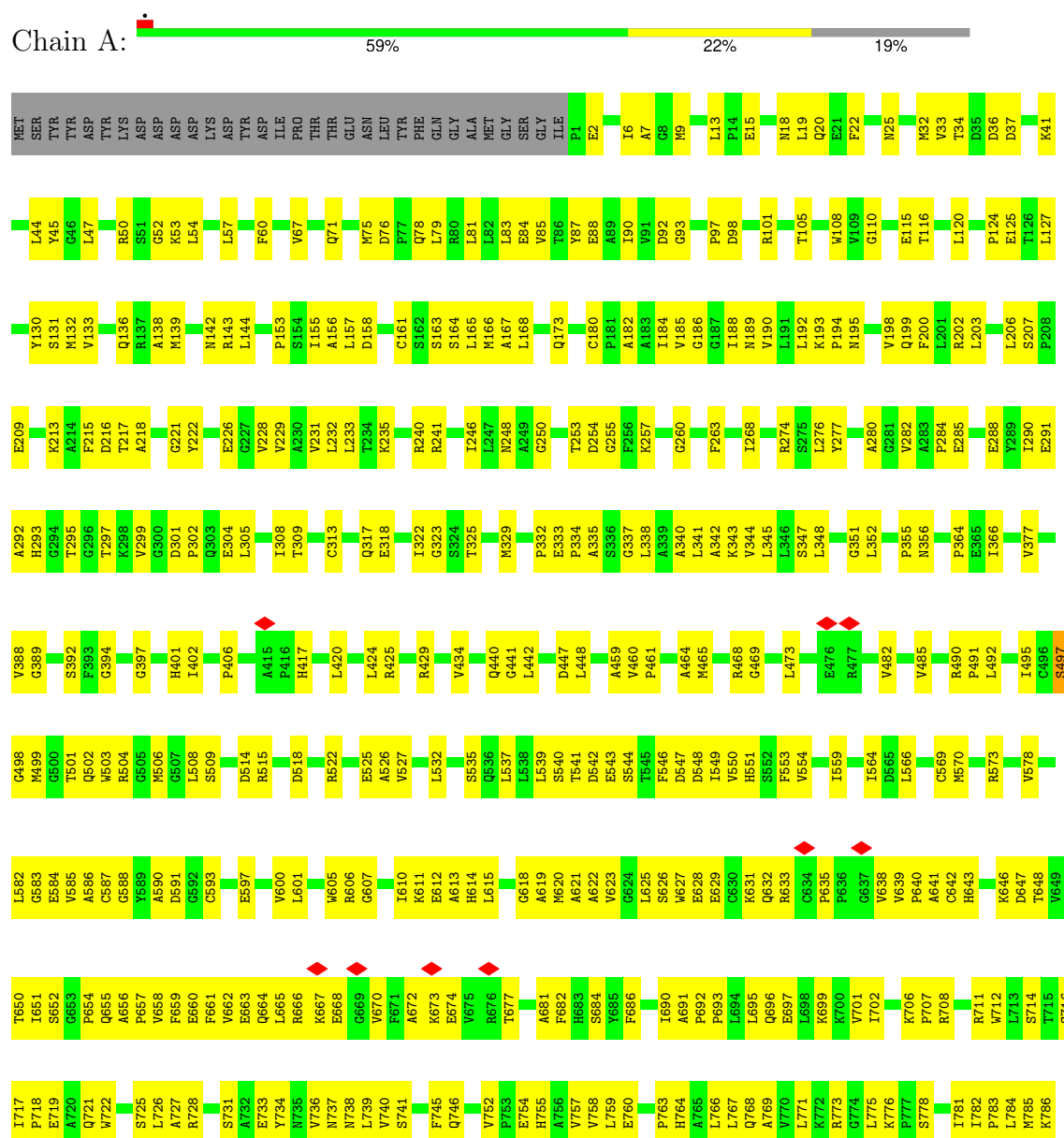


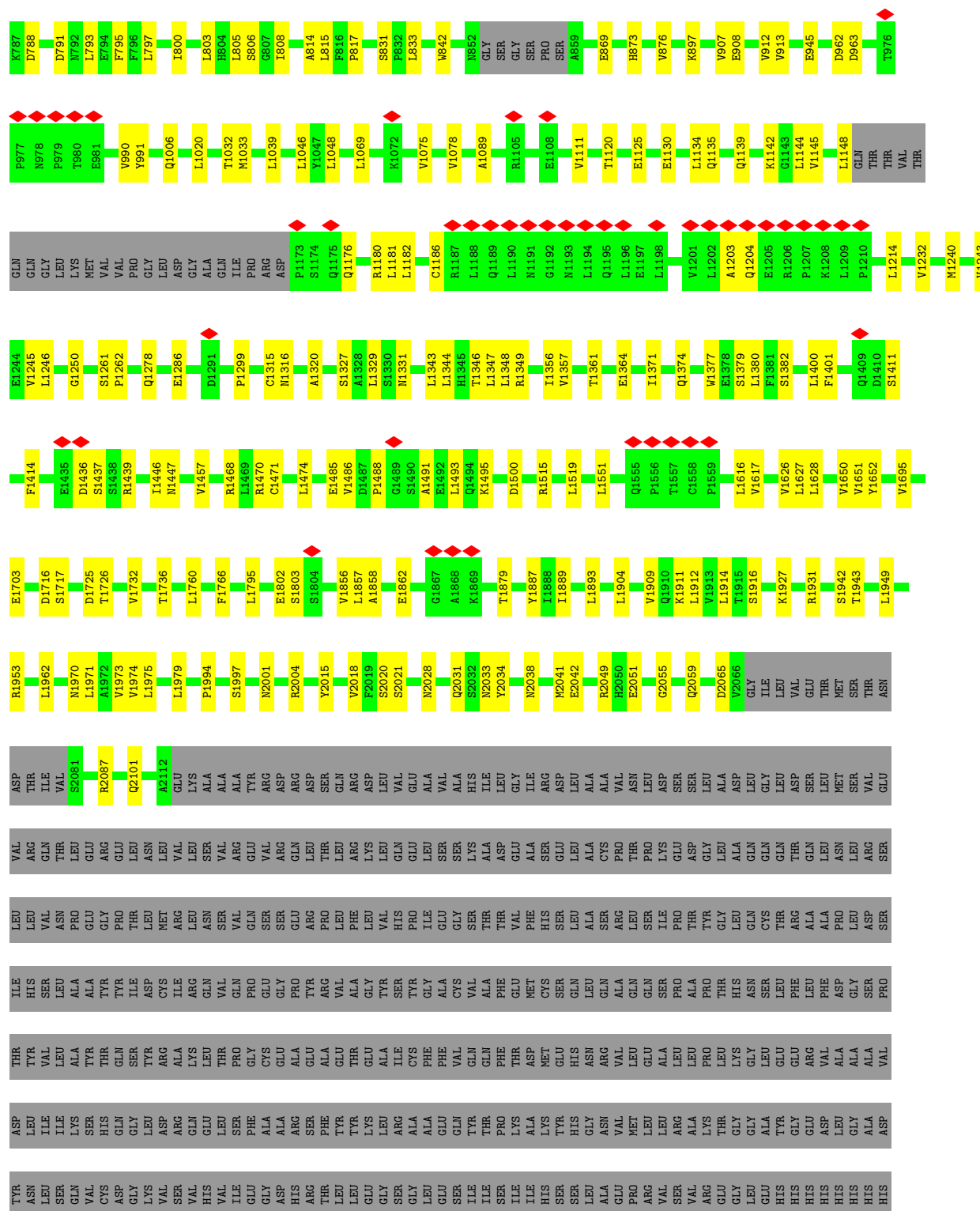
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

### 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: Fatty acid synthase

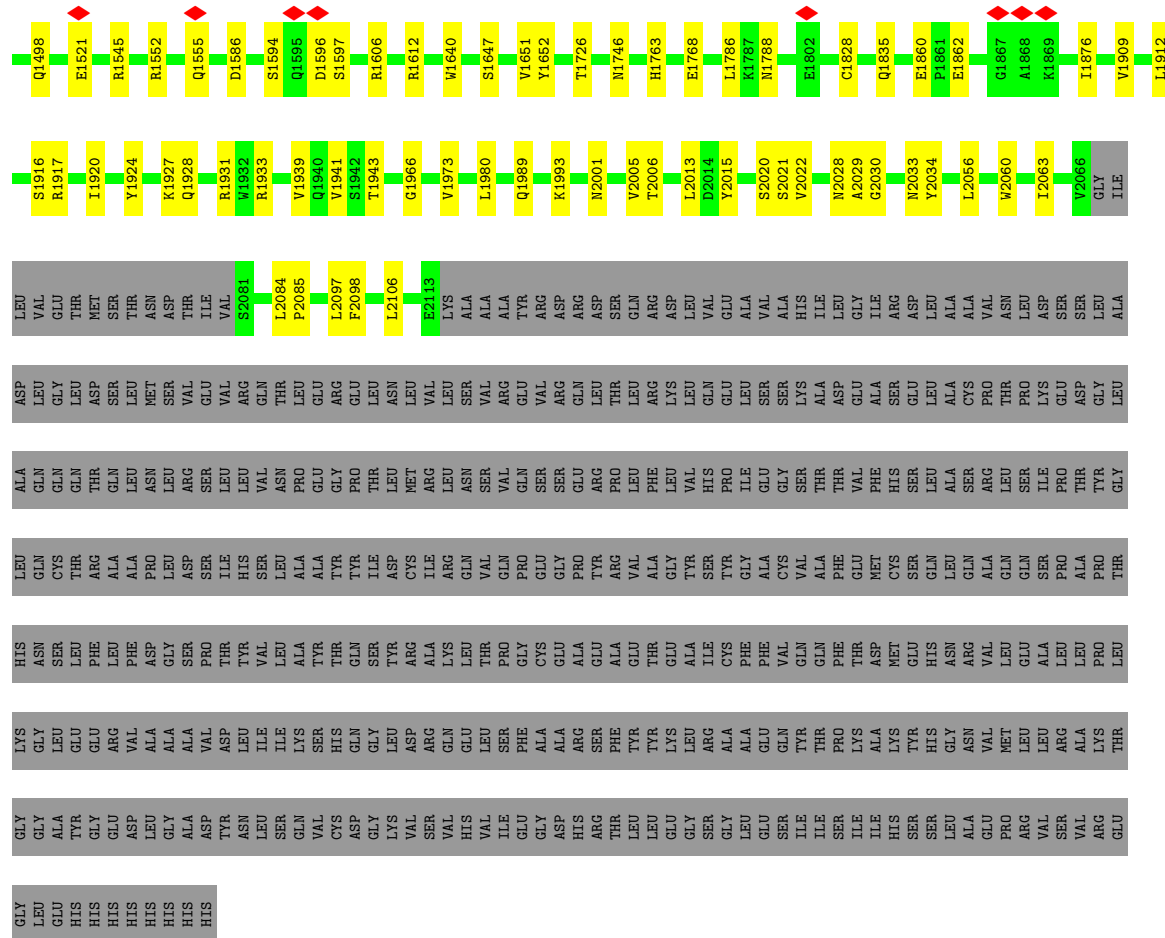




• Molecule 1: Fatty acid synthase



L1307	C1186	P979	A798	W722	Q655	L582	S509	P414	T325	V228	A138	Y45	MET
A1318	R1187	T980	R802	H723	A656	V585	R512	A415	K326	V229	M139	R49	SER
N1331	Q1189	E981	L803	S724	P657	D591	R512	L420	S327	A230	M140	R50	TYR
L1343	L1190	Y991	H804	L726	F659	D592	D514	R425	N328	R51	R143	S51	ASP
L1347	N1191	Q1006	L805	A727	E660	G592	R515	F435	M329	S51	L144	L54	LYS
A1349	S806	G1007	S806	E728	F661	C593	F516	R425	G330	Y242	F160	K55	ASP
I1356	A814	G1007	A814	T729	E662	Q596	R517	R429	H331	Y243	F160	K56	ASP
E1364	L815	L1013	L815	E733	E663	E597	I520	R429	P332	L247	A156	K57	ASP
P1365	L815	E1014	L815	Y734	E664	E598	L521	R429	E333	N248	L157	D56	ASP
Q1366	P822	L1021	P822	W735	L665	E599	L521	V434	A249	A249	A157	S58	ASP
Y1367	A823	L1021	A823	W736	L666	A599	D524	Q435	G250	G250	T159	R59	LYS
Q1200	E824	L1021	E824	W737	K667	L601	E525	Q435	T251	T251	A160	F60	ASP
W1201	P824	L1021	P824	W738	E668	Y604	E525	L438	N252	N252	A160	V67	TYR
Q1202	T827	W1021	T827	W739	G669	W605	A526	L438	D254	D254	C161		ASP
Q1203	P828	W1021	P828	L739	G669	W605	A526	L438	T253	T253	C161		ASP
Q1204	L829	T1032	L829	W740	V670	W605	V527	Q440	L341	L341	S162		PRO
Q1205	L830	Y1047	L830	S741	F671	R606	L532	G441	K343	K343	S163	M75	THR
Q1206	S831	Y1047	S831	W742	A672	G609	K533	L442	V344	V344	L165	D76	THR
Q1207	P832	D1071	P832	W743	E674	L610	V534	D447	L346	L346	M166	P77	GLU
Q1208	L833	K1072	L833	F745	E675	Q536	Q536	F450	S347	S347	A167	Q78	LEU
Q1209	L840	Q1109	L840	Q746	R676	A613	Q536	L451	L348	L348	N170	R80	TYR
Q1210	E848	Q1110	E848	E747	T677	H614	L539	L451	G351	G351	A171	L81	PHE
L1215	N852	V1111	N852	L749	G679	L615	S540	M453	L352	L352	I175	L82	GLN
L1218	GLY	C1141	GLY	E754	M680	P616	T541	M453	A354	A354	Q179	L83	GLY
L1228	SER	Y1145	SER	H755	F682	G618	E543	A459	L276	L276	C180	V85	ALA
D1229	GLY	T1150	GLY	W758	H683	A619	T545	A461	L357	L357	P181	T86	GLY
A1231	LEU	T1150	LEU	L759	H684	A621	F546	A462	H358	H358	E88	E88	SER
V1232	LYS	T1150	LYS	E760	F685	A622	D547	A464	N363	N363	I95	I95	ILE
E1233	MET	T1150	MET	W761	F686	A622	D548	M465	P364	P364	N96	N96	E2
N1234	VAL	T1150	VAL	I761	E687	G624	F549	M465	E365	E365	P97	P97	I6
I1256	VAL	T1150	VAL	A762	E688	L625	V550	R468	I366	I366	D98	D98	
S1261	GLY	T1150	GLY	P763	A689	S626	F553	Q469	L369	L369	R101	R101	M9
P1282	ASP	T1150	ASP	L767	I690	W627	V554	Q469	G372	G372	H104	H104	L13
A1272	ALA	T1150	ALA	Q768	A691	E628	S555	E476	A291	A291	T105	T105	P14
T1273	GLN	T1150	GLN	A769	P692	E629	L556	R477	H293	H293	V198	V198	
D1274	ILE	T1150	ILE	L771	P693	G630	T557	V452	G294	G294	Q199	Q199	L19
R1275	ARG	T1150	ARG	L775	L694	K631	A558	V452	T295	T295	W108	W108	
Q1278	ASP	T1150	ASP	K776	E697	G634	Q630	V452	G296	G296	R202	R202	F22
E1286	S1173	T1150	S1173	L777	V701	P635	Q630	V452	T297	T297	S207	S207	W23
L1287	Q1174	T1150	L1287	W778	I702	P635	I561	R490	E304	E304	E115	E115	L26
Q1288	Q1175	T1150	Q1288	T780	K706	P635	D565	P491	L305	L305	E115	E115	L27
Q1289	E1177	T1150	Q1289	I781	P707	P635	L566	W493	G394	G394	L120	L120	M32
V1292		T1150	V1292	I782	R708	P635	C569	F494	F395	F395	D216	D216	V33
G1295		T1150	G1295	W784	L713	P635	P574	I495	G396	G396	T217	T217	T34
A1300		T1150	A1300	W785	S714	P635	D575	C497	H401	H401	G221	G221	D35
		T1150		K786	S716	P635	G576	C497	V400	V400	Y222	Y222	D36
		T1150		K787	T717	P635	I577	C497	L404	L404	L127	L127	D37
		T1150		L793	I717	P635	V578	C497	Q502	Q502	S131	S131	R38
		T1150		L797	P718	P635	G579	C497	W503	W503	M132	M132	R39
		T1150			E719	P635	V581	C497	N407	N407	E226	E226	
		T1150			A720	P635	S581	C497	Q409	Q409	G227	G227	L44



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	116738	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	0.734	Depositor
Minimum map value	-0.214	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.193	Depositor
Map size ( $\text{\AA}$ )	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 ( $\text{\AA}$ )	1.069, 1.069, 1.069	Depositor

## 5 Model quality

### 5.1 Standard geometry

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	0.25	0/16198	0.47	0/22023
1	B	0.25	0/16222	0.48	0/22055
All	All	0.25	0/32420	0.47	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

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	521	0
1	B	15857	9380	15826	479	0
2	A	96	52	52	4	0
2	B	96	52	52	2	0
All	All	31882	18827	31739	982	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 982 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:622:ALA:HA	1:A:650:THR:HA	1.37	1.06
1:B:619:ALA:HB3	1:B:658:VAL:HG11	1.35	1.03
1:B:767:LEU:HB3	1:B:771:LEU:HD23	1.37	1.02
1:B:78:GLN:HB3	1:B:188:ILE:HD12	1.44	0.99
1:B:1989:GLN:O	1:B:1993:LYS:HG3	1.62	0.98

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	2060/2553 (81%)	2010 (98%)	50 (2%)	0	100	100
1	B	2063/2553 (81%)	2019 (98%)	44 (2%)	0	100	100
All	All	4123/5106 (81%)	4029 (98%)	94 (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	1705/2117 (80%)	1703 (100%)	2 (0%)	92	96
1	B	1708/2117 (81%)	1706 (100%)	2 (0%)	92	96
All	All	3413/4234 (81%)	3409 (100%)	4 (0%)	92	96

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	497	SER
1	A	734	TYR
1	B	293	HIS
1	B	1924	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 29 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1555	GLN
1	B	2001	ASN
1	B	170	ASN
1	B	1345	HIS
1	B	142	ASN

### 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	B	2602	-	47,52,52	0.67	0	61,80,80	0.79	2 (3%)
2	NDP	B	2601	-	47,52,52	0.63	0	61,80,80	0.85	2 (3%)
2	NDP	A	2601	-	47,52,52	0.66	0	61,80,80	0.78	3 (4%)
2	NDP	A	2602	-	47,52,52	0.66	0	61,80,80	0.85	2 (3%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	B	2602	-	-	8/30/77/77	0/5/5/5
2	NDP	B	2601	-	-	10/30/77/77	0/5/5/5
2	NDP	A	2601	-	-	13/30/77/77	0/5/5/5
2	NDP	A	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	A	2602	NDP	P2B-O2B-C2B	-3.94	112.91	123.43
2	B	2601	NDP	P2B-O2B-C2B	-3.52	114.04	123.43
2	B	2602	NDP	P2B-O2B-C2B	-3.49	114.12	123.43
2	B	2601	NDP	C5A-C6A-N6A	2.41	123.99	120.31
2	A	2601	NDP	C4B-O4B-C1B	-2.30	107.81	109.92

There are no chirality outliers.

5 of 41 torsion outliers are listed below:

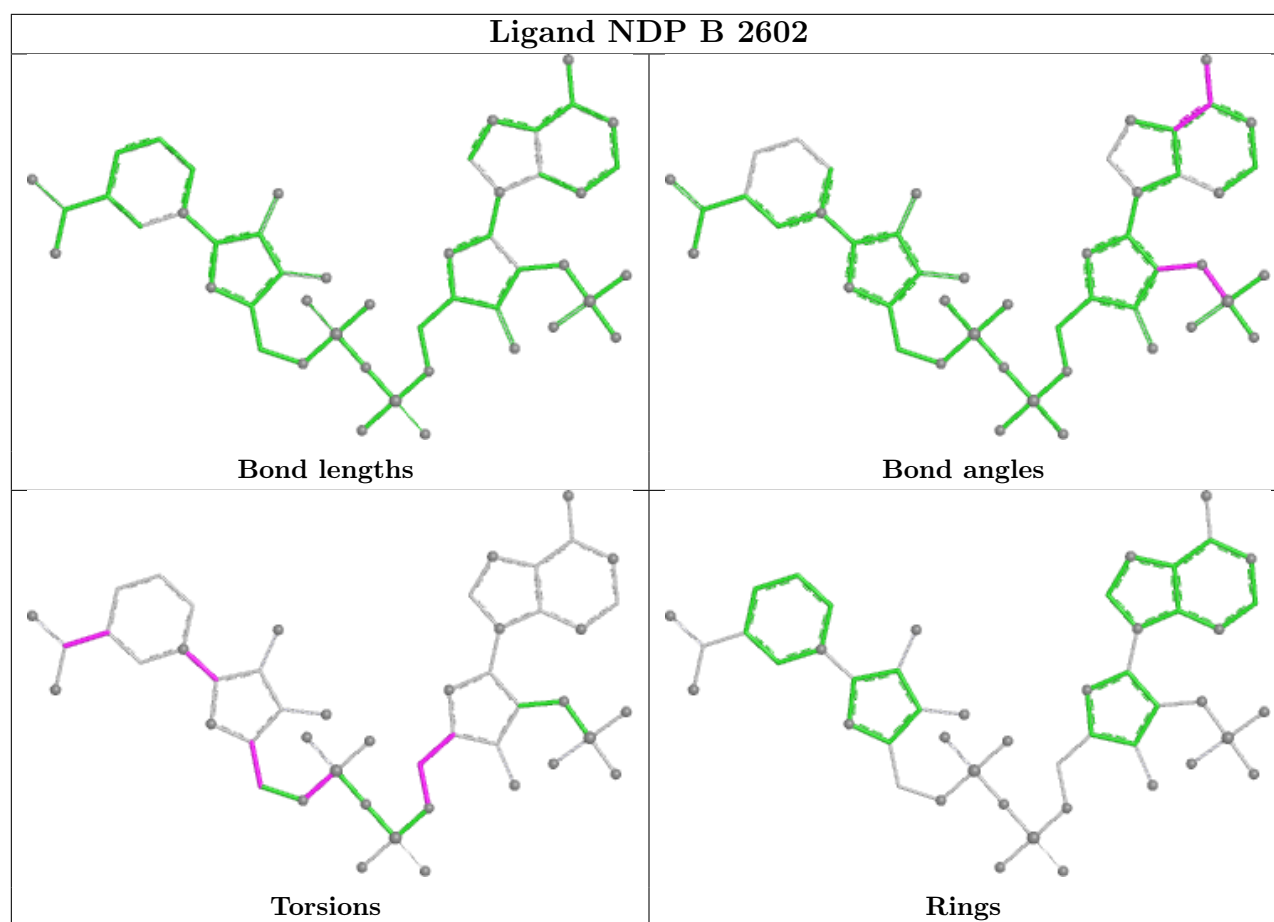
Mol	Chain	Res	Type	Atoms
2	A	2601	NDP	C5D-O5D-PN-O3
2	A	2601	NDP	C5D-O5D-PN-O1N
2	A	2601	NDP	C2N-C3N-C7N-N7N
2	A	2602	NDP	C5D-O5D-PN-O3
2	A	2602	NDP	C5D-O5D-PN-O2N

There are no ring outliers.

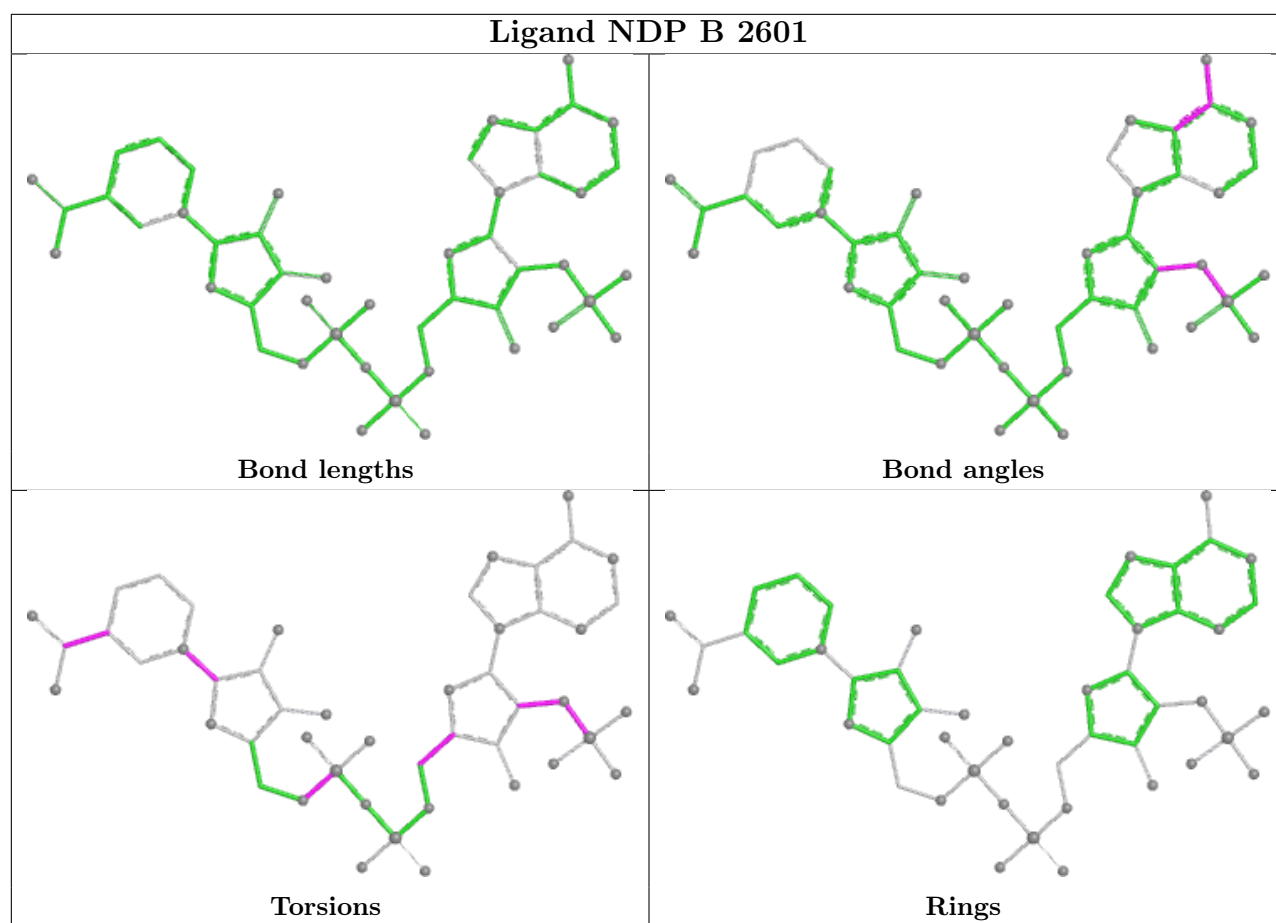
3 monomers are involved in 6 short contacts:

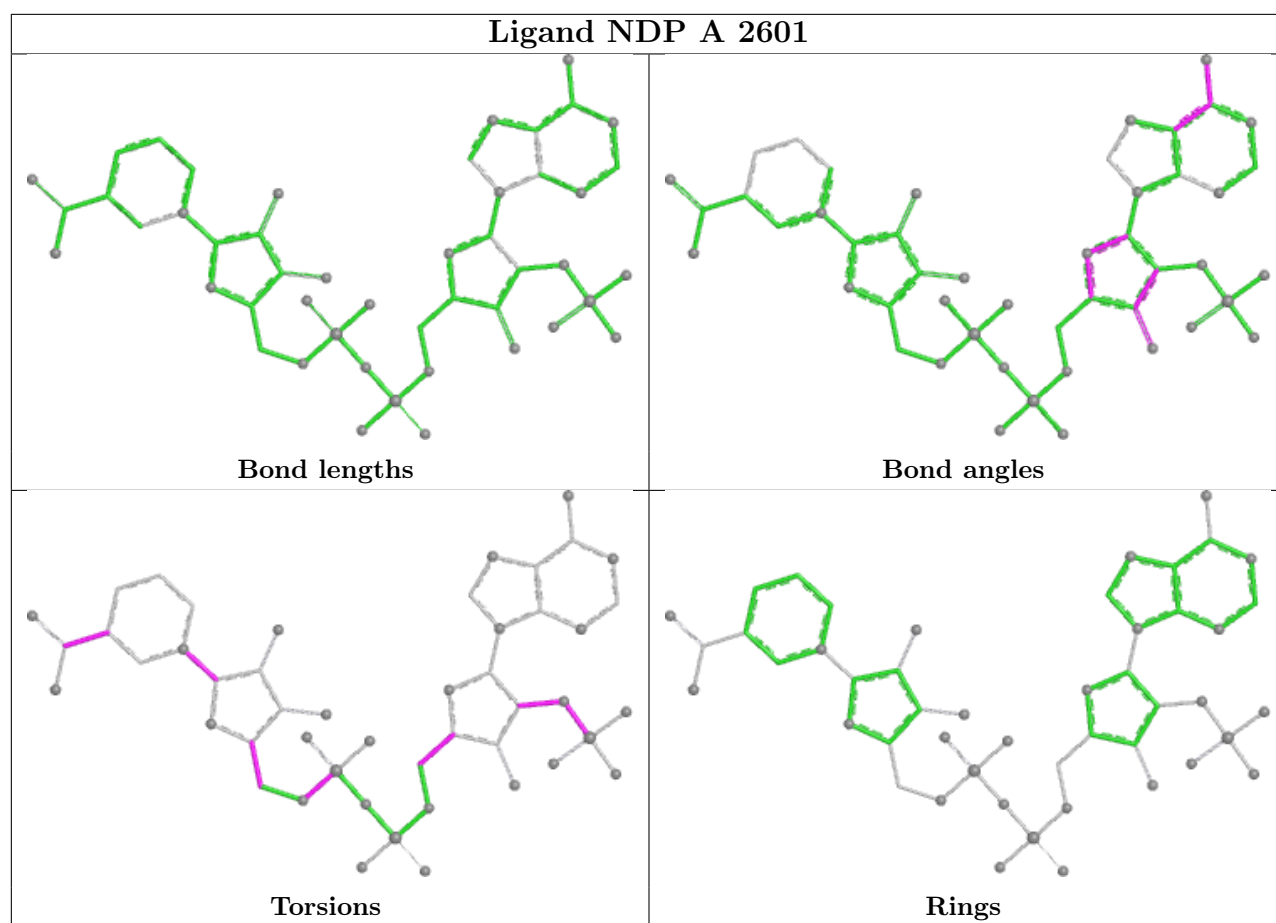
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2602	NDP	2	0
2	A	2601	NDP	1	0
2	A	2602	NDP	3	0

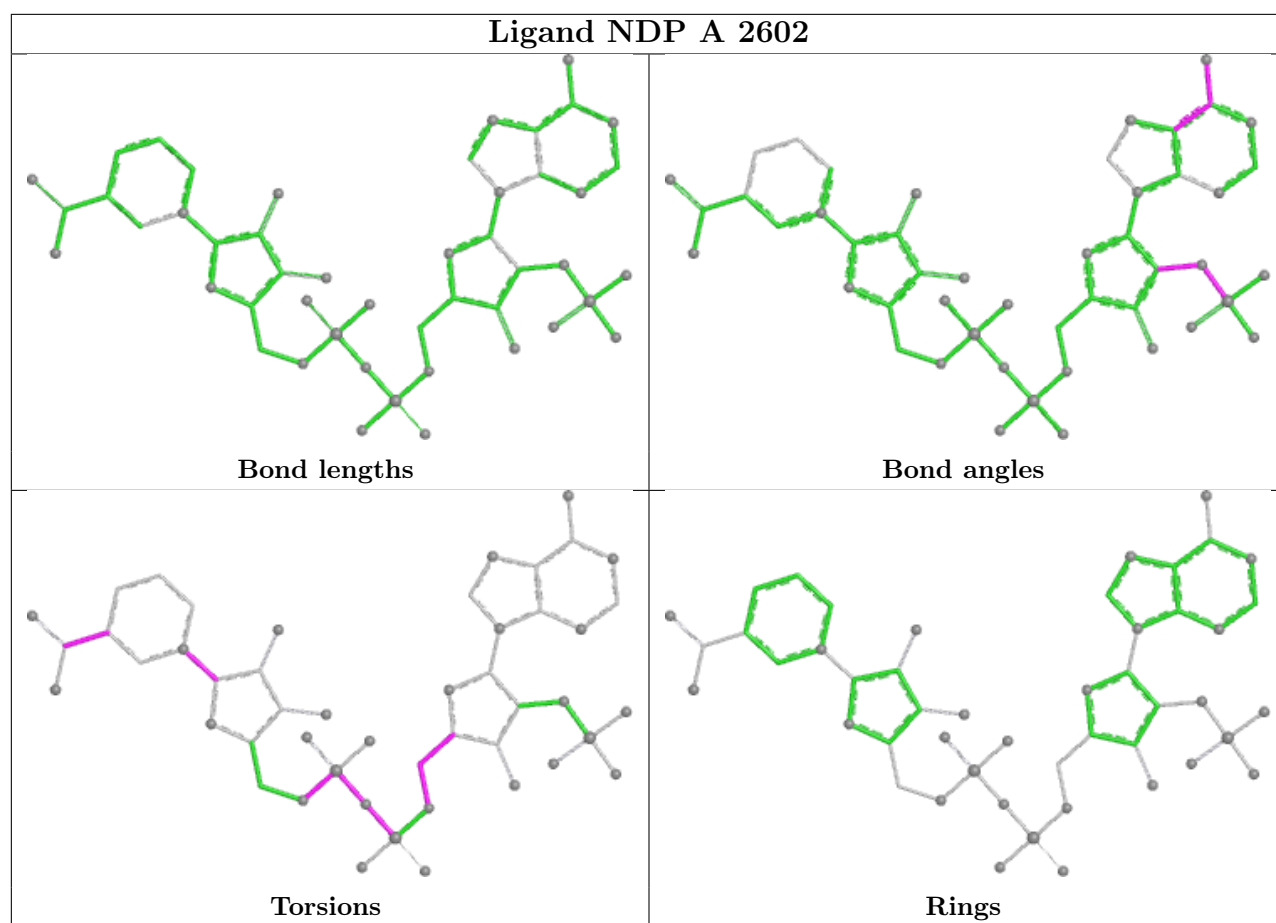
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

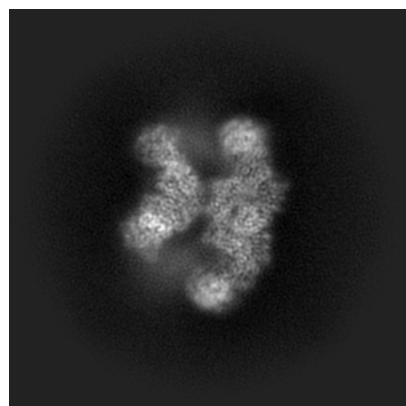
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43354. These allow visual inspection of the internal detail of the map and identification of artifacts.

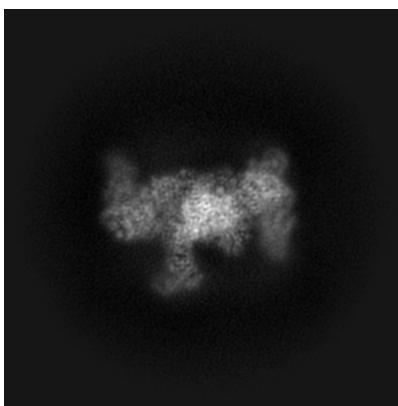
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

### 6.1 Orthogonal projections [i](#)

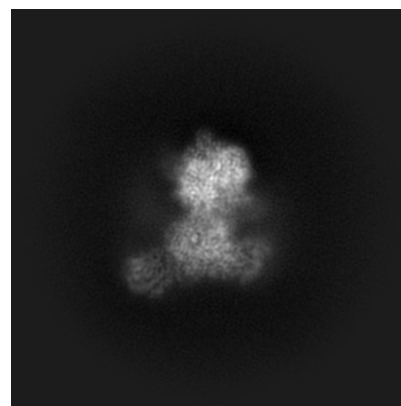
#### 6.1.1 Primary map



X

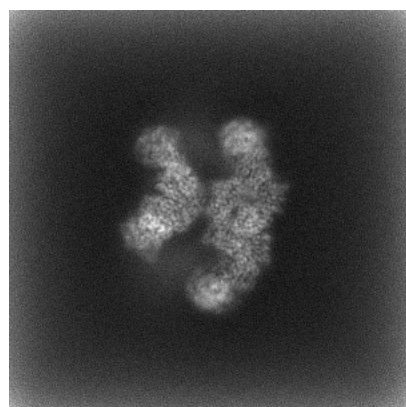


Y

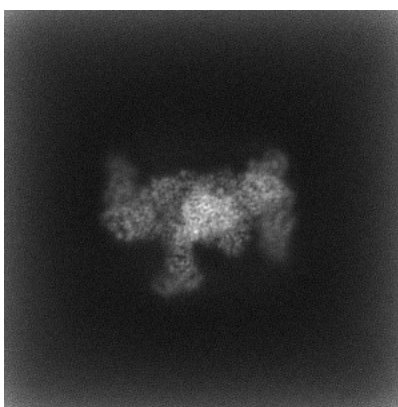


Z

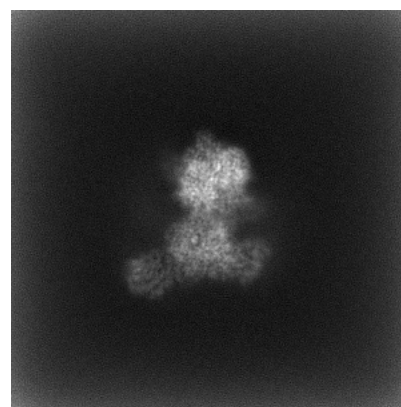
#### 6.1.2 Raw map



X



Y

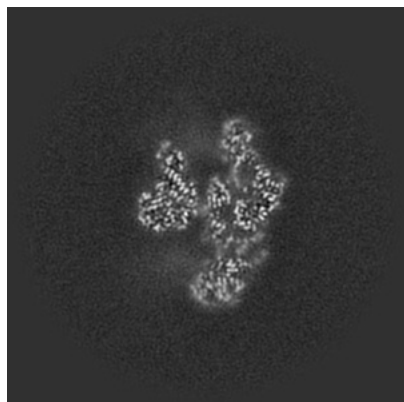


Z

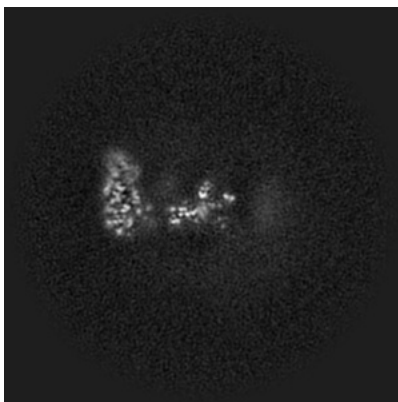
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

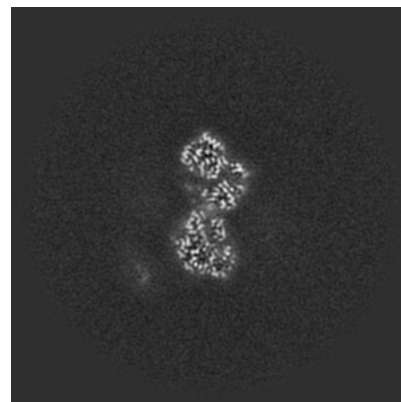
### 6.2.1 Primary map



X Index: 180

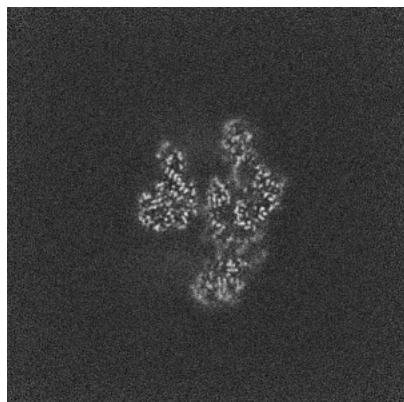


Y Index: 180



Z Index: 180

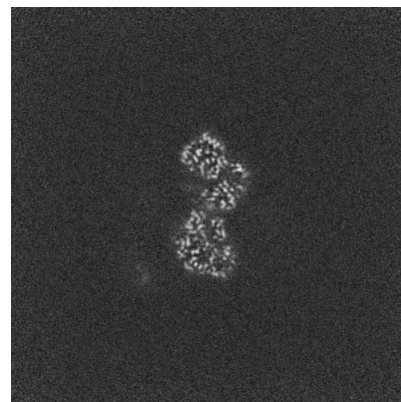
### 6.2.2 Raw map



X Index: 180



Y Index: 180

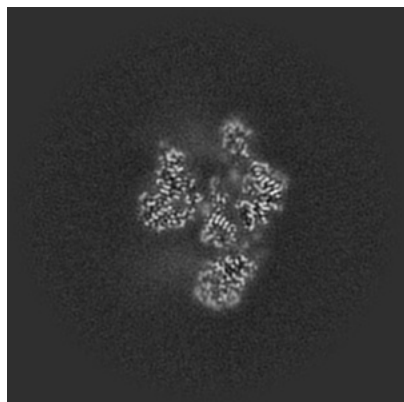


Z Index: 180

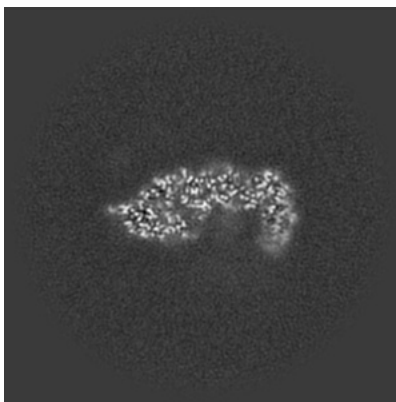
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

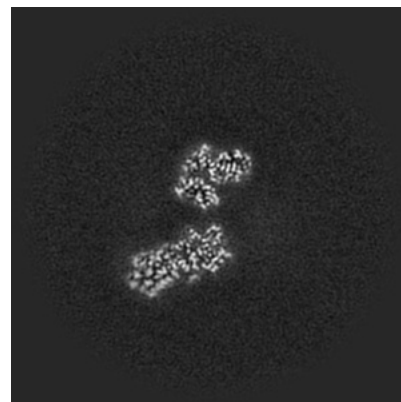
### 6.3.1 Primary map



X Index: 177

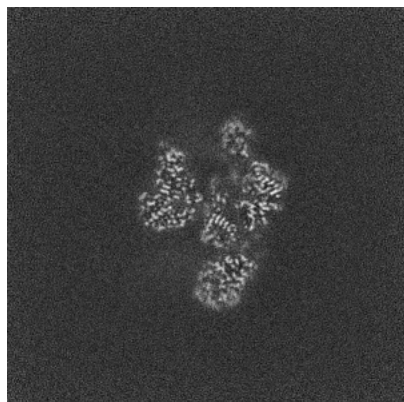


Y Index: 207



Z Index: 165

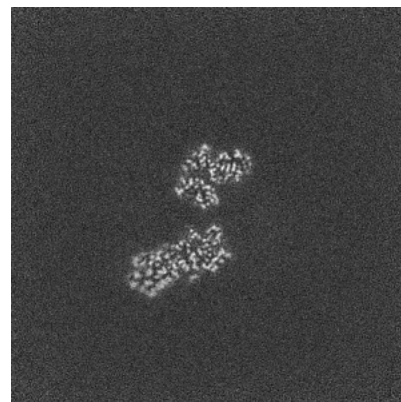
### 6.3.2 Raw map



X Index: 177



Y Index: 217



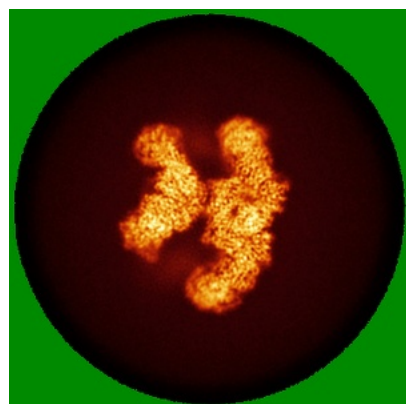
Z Index: 165

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

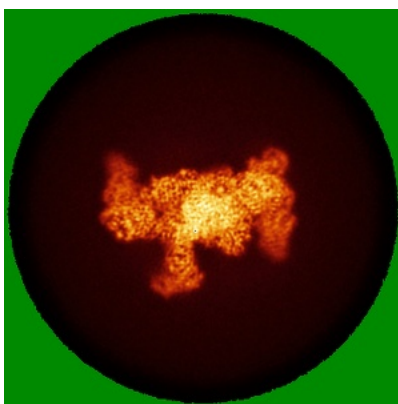


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

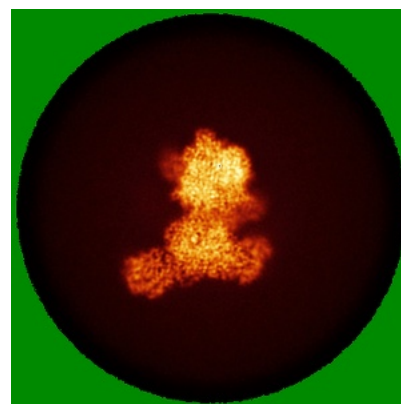
### 6.4.1 Primary map



X

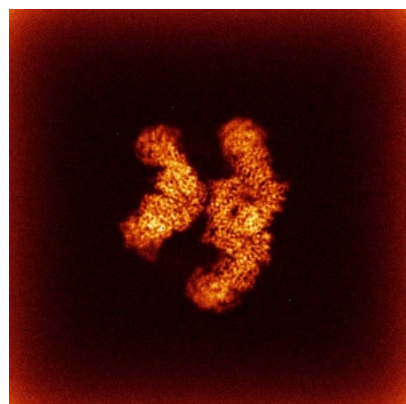


Y

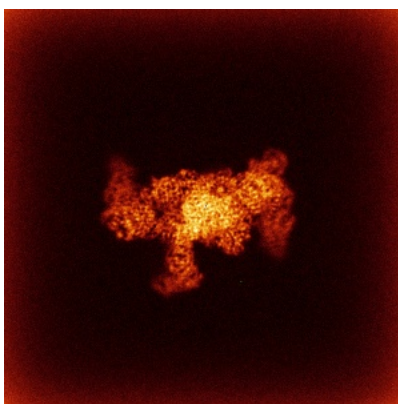


Z

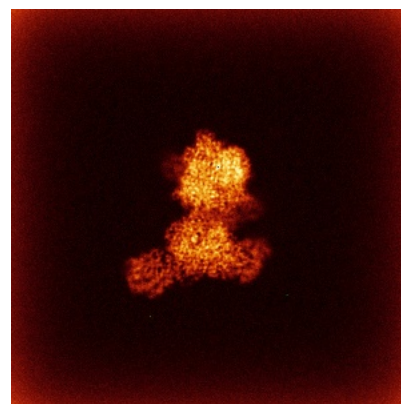
### 6.4.2 Raw map



X



Y

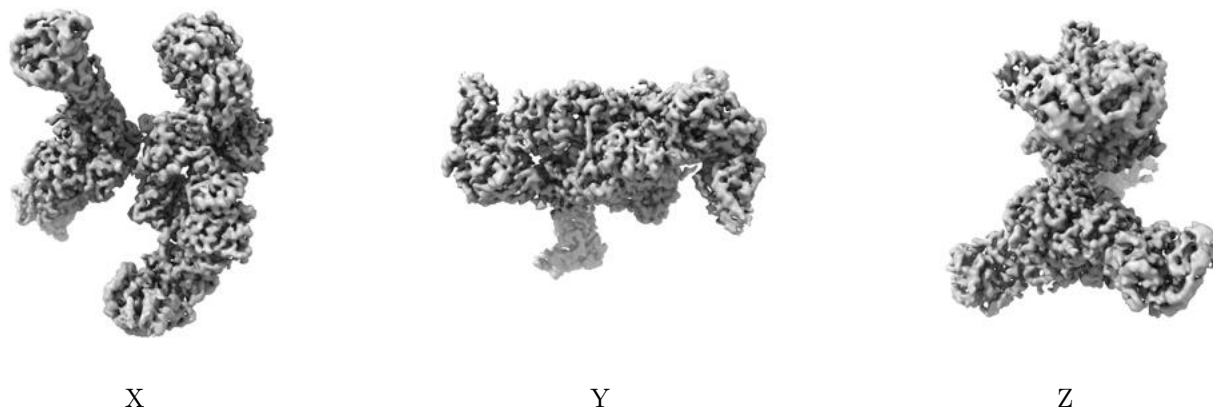


Z

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.

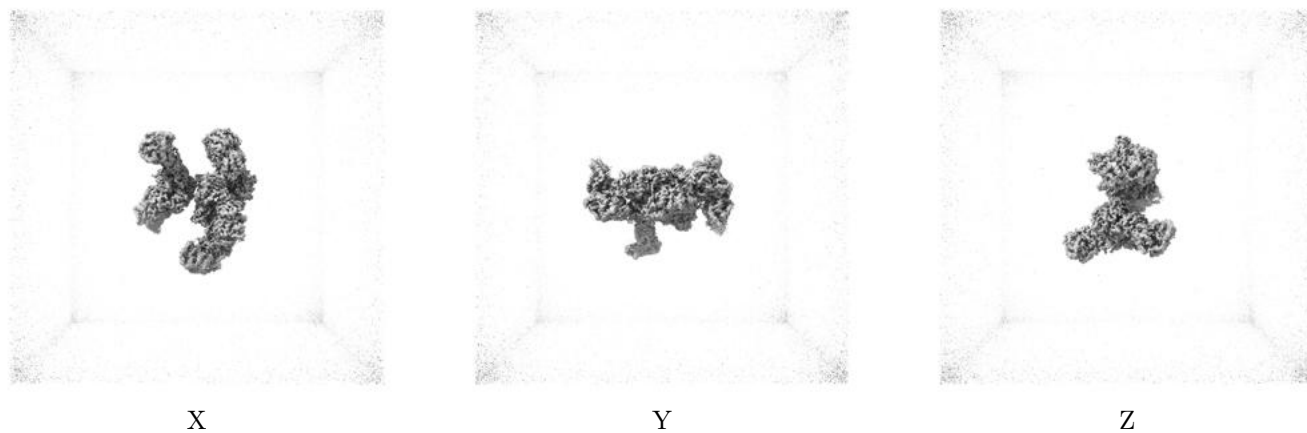
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.193. 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.



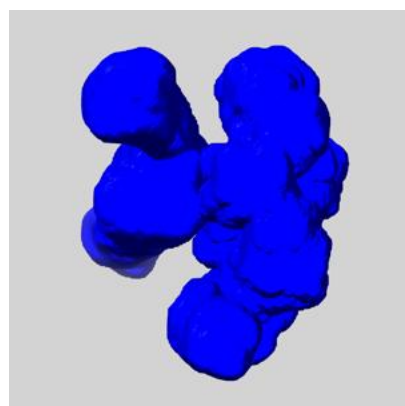
## 6.6 Mask visualisation [i](#)

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

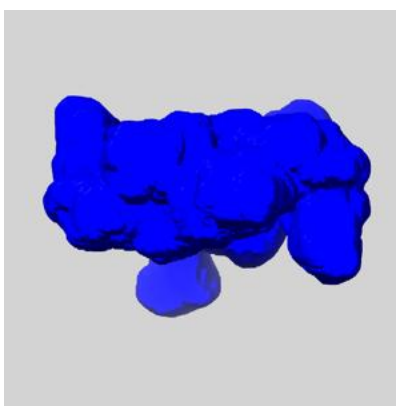
A mask typically either:

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

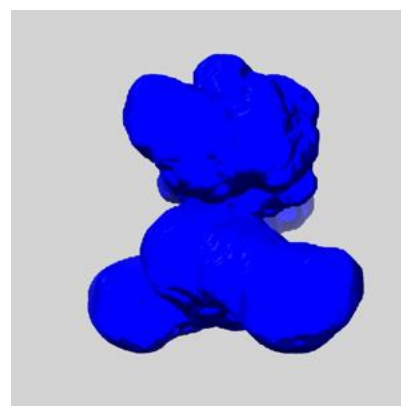
### 6.6.1 emd\_43354\_msk\_1.map [i](#)



X



Y

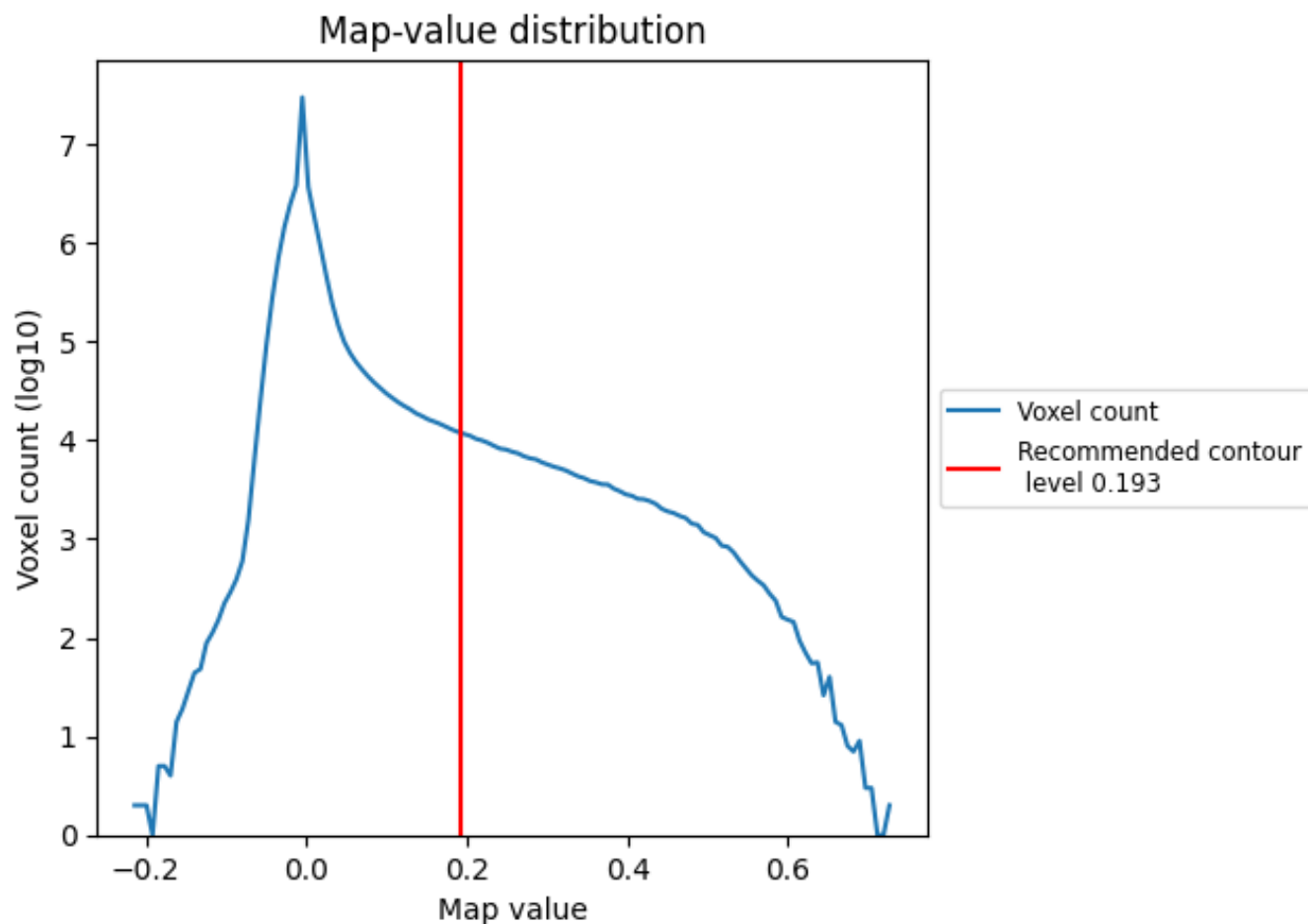


Z

## 7 Map analysis [i](#)

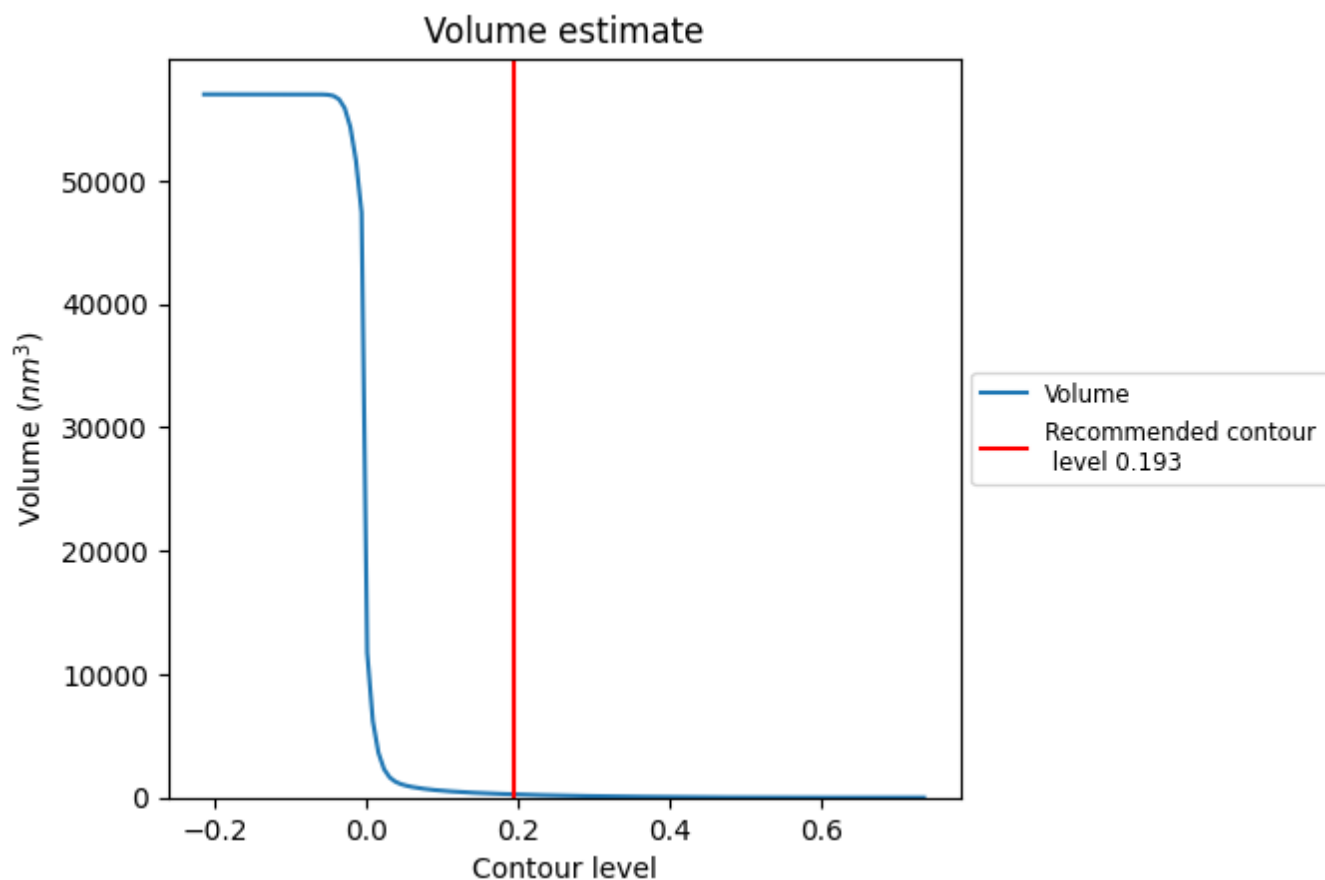
This section contains the results of statistical analysis of the map.

### 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.

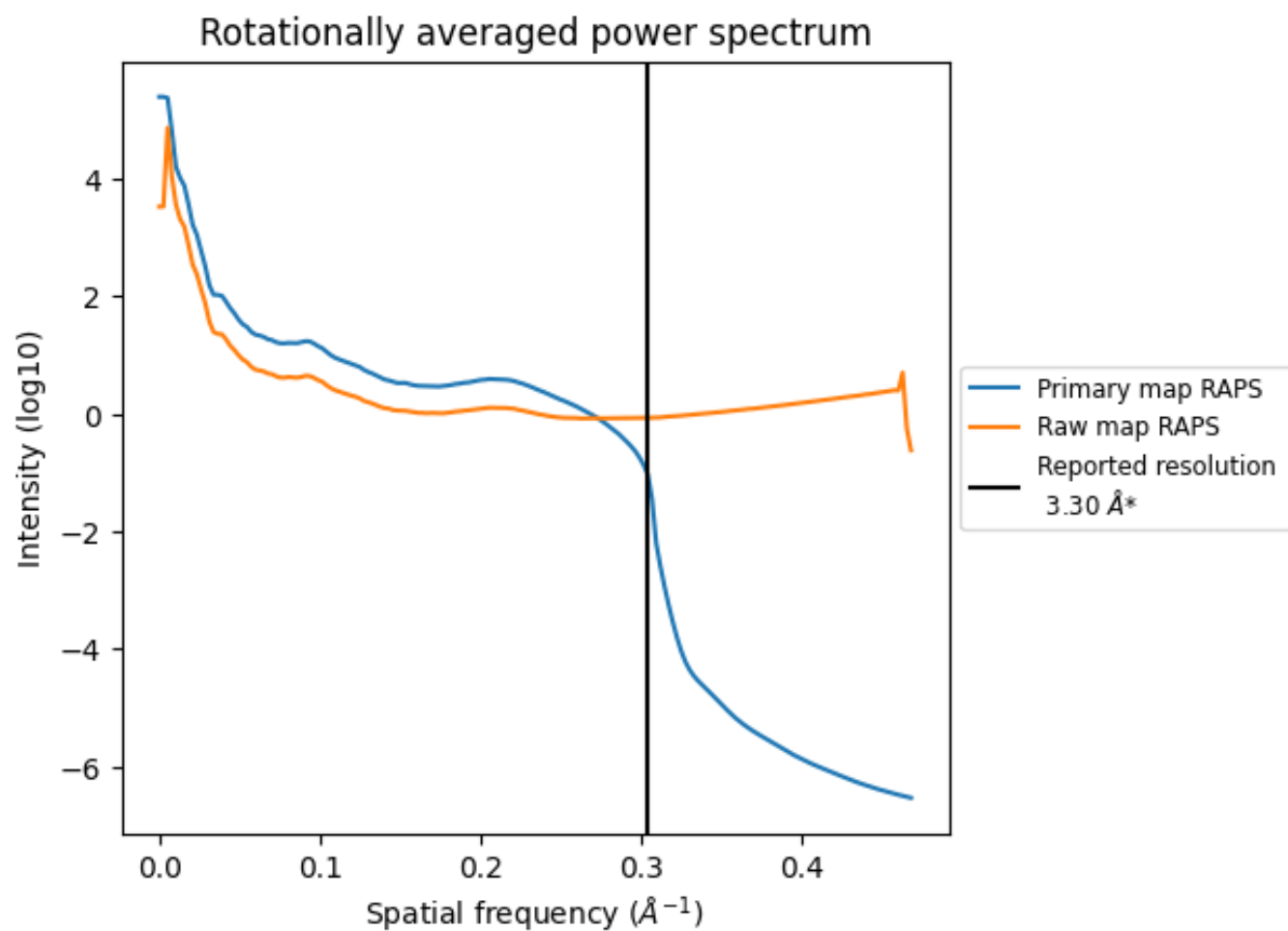
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 263 nm<sup>3</sup>; this corresponds to an approximate mass of 237 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 ⓘ

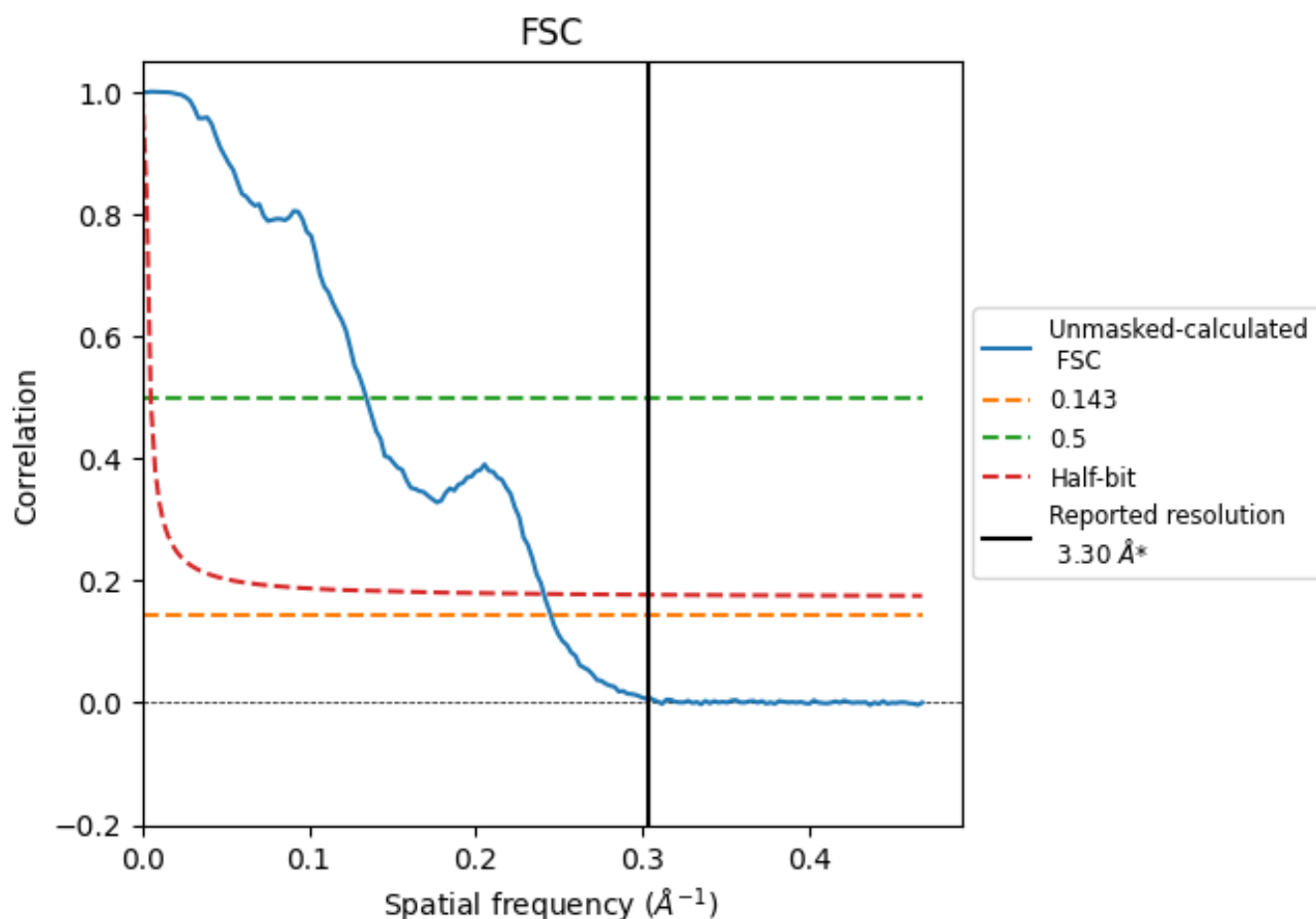


\*Reported resolution corresponds to spatial frequency of  $0.303 \text{ \AA}^{-1}$

## 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 0.303 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

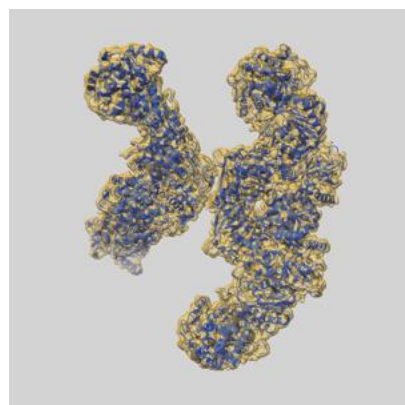
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.08	7.45	4.15

\*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 4.08 differs from the reported value 3.3 by more than 10 %

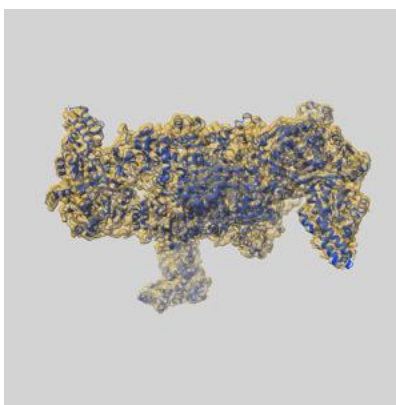
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43354 and PDB model 8VM7. Per-residue inclusion information can be found in section [3](#) on page [7](#).

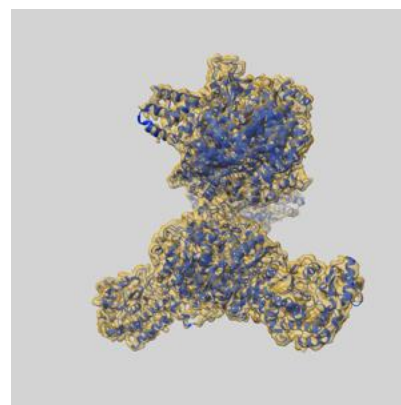
### 9.1 Map-model overlay [i](#)



X



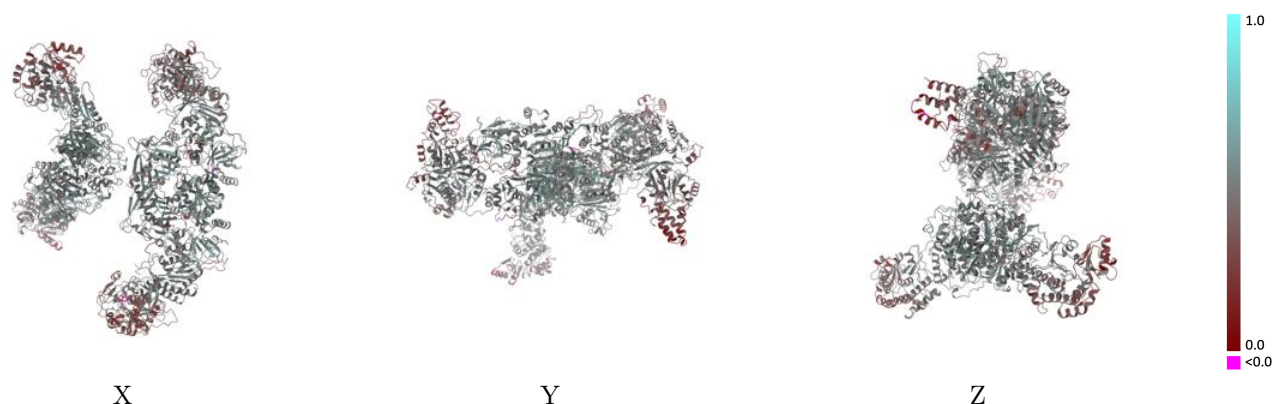
Y



Z

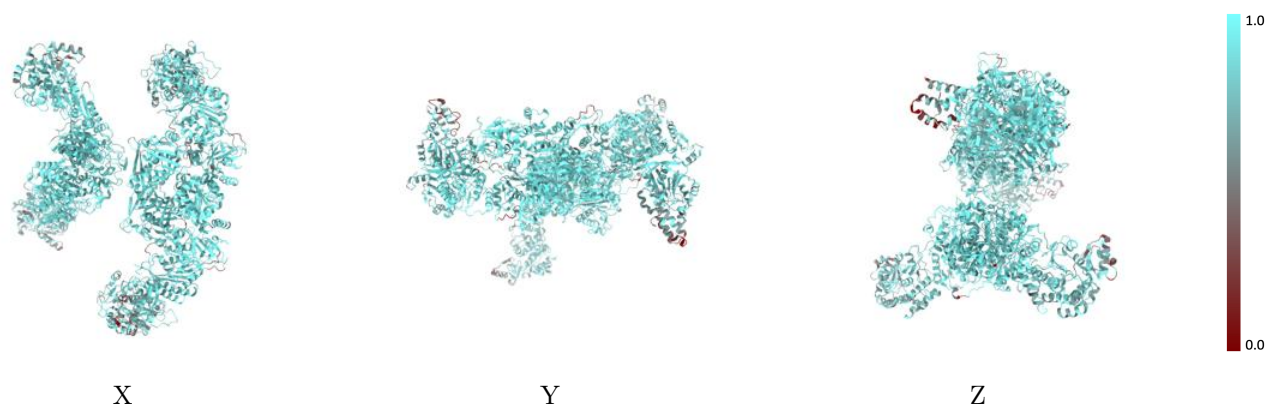
The images above show the 3D surface view of the map at the recommended contour level 0.193 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

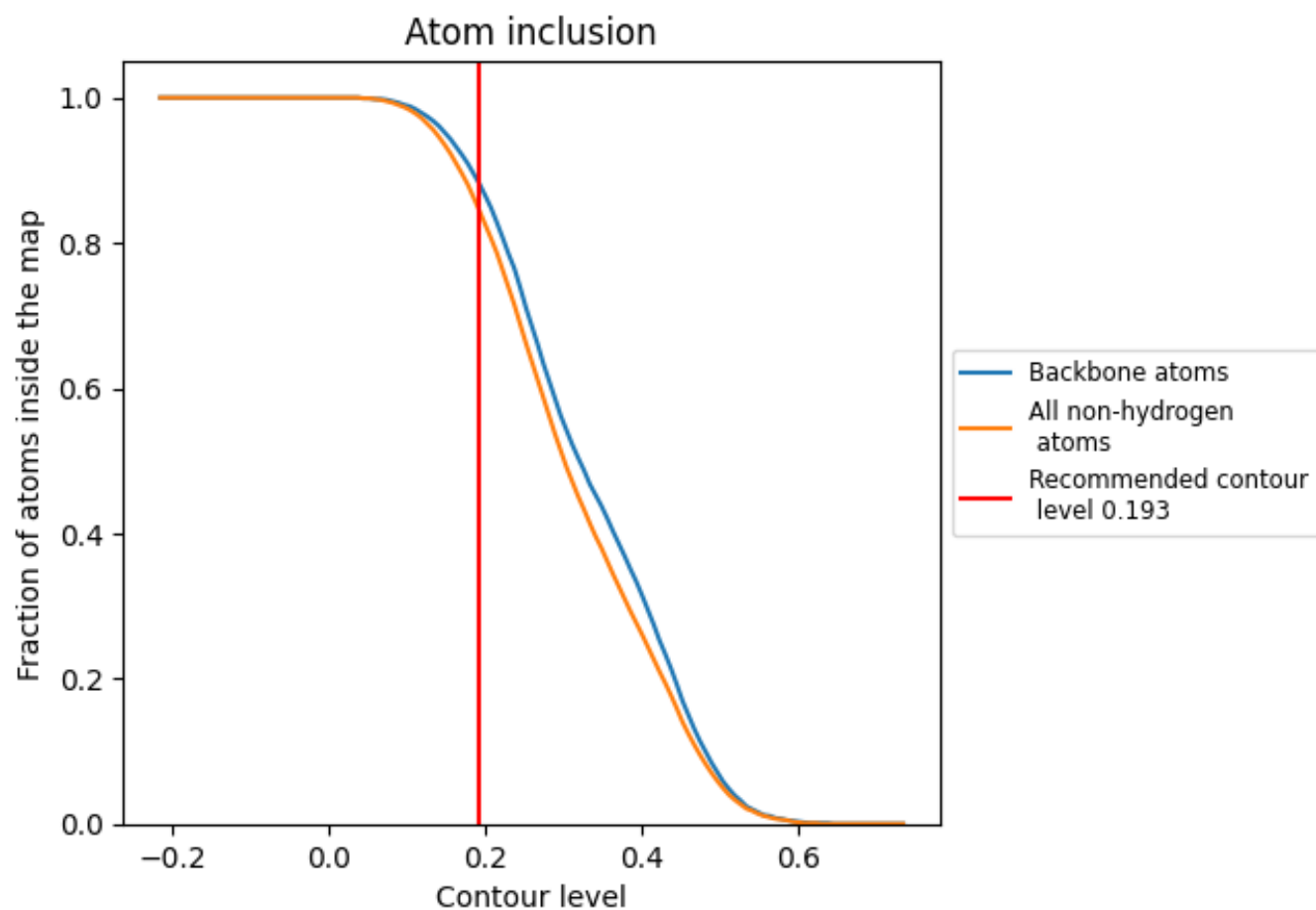
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.193).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 88% of all backbone atoms, 84% 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 (0.193) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.8450	<div></div> 0.4630
A	<div></div> 0.8490	<div></div> 0.4640
B	<div></div> 0.8410	<div></div> 0.4620

