



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 12:46 PM UTC

PDB ID : 8VLE / pdb_00008vle
EMDB ID : EMD-43337
Title : Composite structure of human FASN with NADPH in State 1
Authors : Schultz, K.; Marmorstein, R.
Deposited on : 2024-01-11
Resolution : 3.30 Å(reported)
Based on initial models : ., 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:

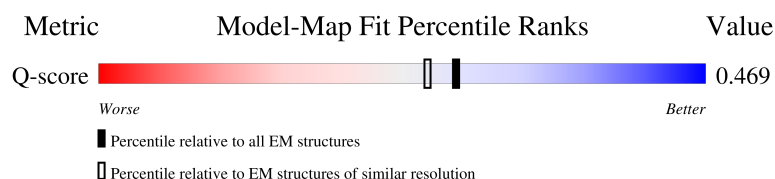
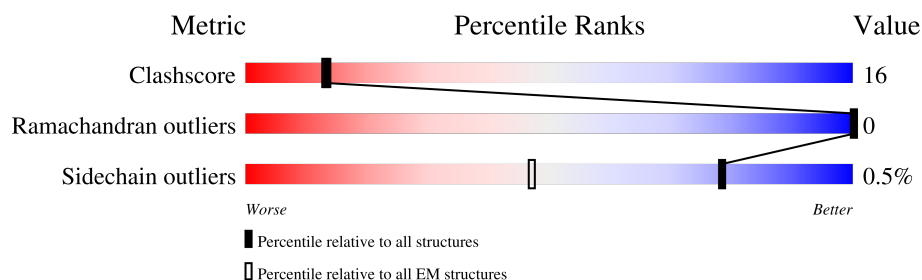
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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	2553	 59% 22% 19%
1	B	2553	 59% 22% 19%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 50715 atoms, of which 18833 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
			25182	10041	9349	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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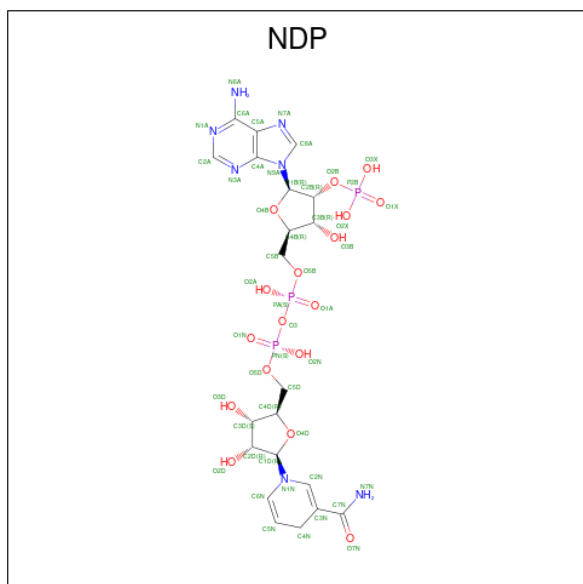
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP P49327
A	-4	MET	-	expression tag	UNP P49327
A	-3	GLY	-	expression tag	UNP P49327
A	-2	SER	-	expression tag	UNP P49327
A	-1	GLY	-	expression tag	UNP P49327
A	0	ILE	-	expression tag	UNP P49327
A	1	PRO	-	expression tag	UNP P49327
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 (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

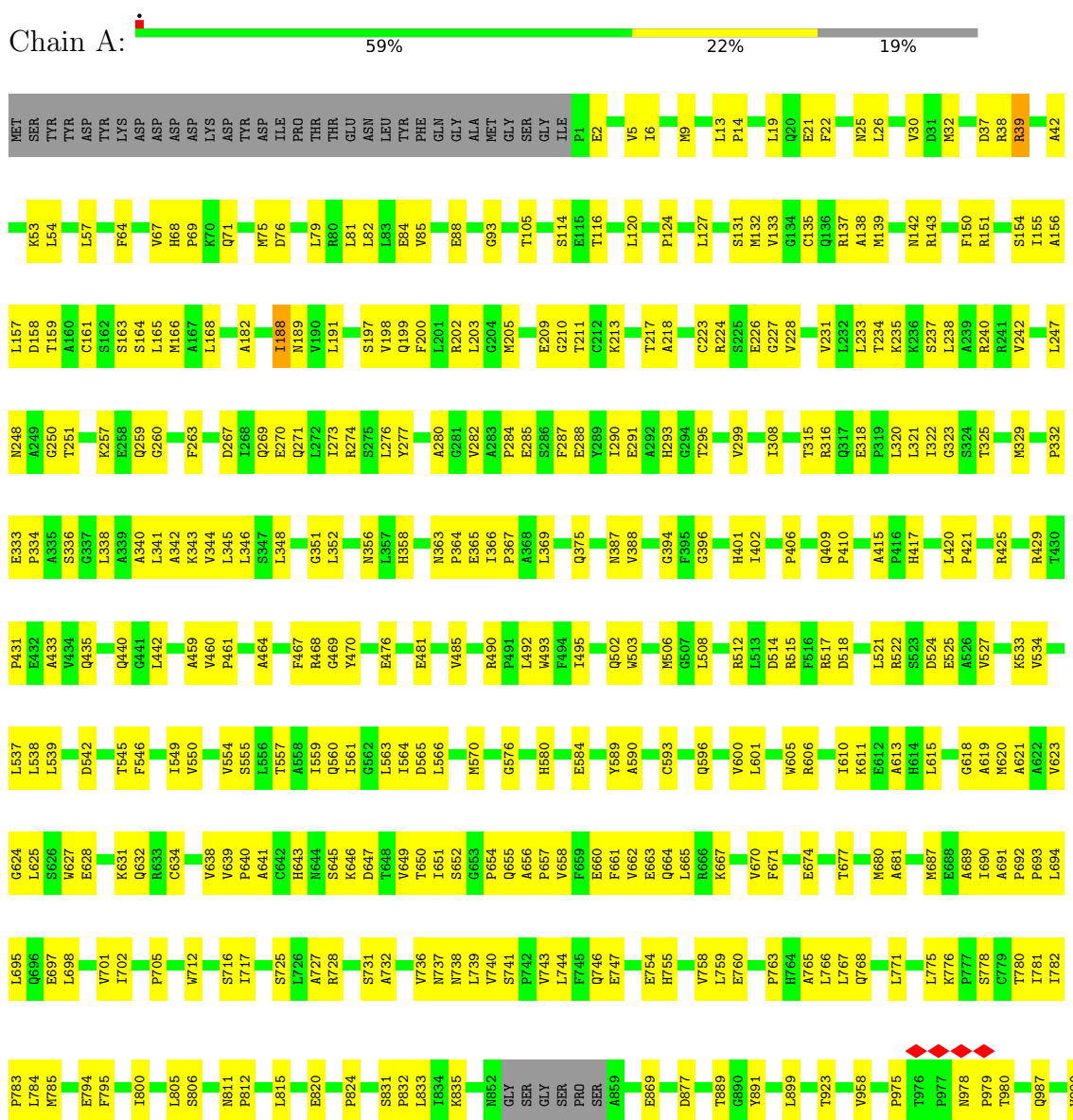


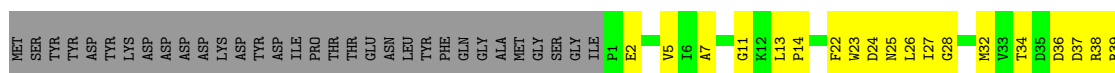
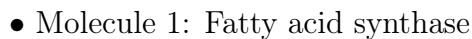
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

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





D1596	S1597	E1602	D1607	A1608	L1616	L1622	F1632	L1633	W1634	V1650	V1651	Y1652	S1677	Q1682	V1699	L1708	L1760	H1763	F1766	D1773	H1778	N1788	D1797	A1798	F1799	F1800	N1801	E1802	H1807	R1808	W1811	V1814	R1824	K1827	E1837	Q1595																			
Y1396	C1403	V1417	D1418	D1419	R1423	K1429	R1439	L1443	K1444	A1445	I1446	V1457	R1461	R1468	L1469	C1470	L1474	D1487	S1490	L1497	L1501	V1502	E1521	S1549	R1552	Q1555	P1556	L1571	N1572	F1573	D1586	P1589	T1593	S1594	Q1595																				
G1250	I1256	Y1270	T1271	A1272	T1273	R1275	L1280	V1292	A1293	Q1294	P1299	L1313	V1314	C1315	N1316	S1327	N1331	L1343	L1344	L1348	L1353	I1356	V1357	T1361	S1362	T1363	E1364	P1365	Q1366	Q1369	G1370	I1371	L1372	S1373	Q1374	A1376	L1386	V1389	G1390	L1391	K1392														
THR	VAL	THR	GLN	GLY	LEU	LYS	MET	VAL	VAL	PRO	GLY	LEU	ASP	GLY	ALA	GLN	ILE	PRO	ARG	ASP	P1173	E1177	L1178	L1190	N1191	G1192	N1193	L1194	Q1195	L1196	E1197	L1198	A1199	L1202	A1203	Q1204	E1205	R1206	L1209	K1208	L1210	L1214	L1215	L1228	D1229	T1230	N1234	V1245	L1246						
A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494	I495	R496	S497	G597	L577	V578	H580	S581	L582	G583	E584	V585	A586	C587	G588	Y589	A590	D591	Q596	A599	V600	R606	T610	K611	L615	M620	A621	A622	V623
G694	L625	G626	W627	E628	E629	C630	K631	G632	R633	C634	P635	V639	P640	G642	H643	M644	S645	K646	D647	T648	V649	T650	R651	P654	Q655	A656	P657	V658	F659	E660	S661	V662	E663	Q664	L665	R666	K667	E668	G669	V670	F671	A672	K673	E674	M680	A681	F682	H683	S684	V685	F686	M687	E688	A689	I690
A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494	I495	R496	S497	G597	L577	V578	H580	S581	L582	G583	E584	V585	A586	C587	G588	Y589	A590	D591	Q596	A599	V600	R606	T610	K611	L615	M620	A621	A622	V623
A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494	I495	R496	S497	G597	L577	V578	H580	S581	L582	G583	E584	V585	A586	C587	G588	Y589	A590	D591	Q596	A599	V600	R606	T610	K611	L615	M620	A621	A622	V623
A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494	I495	R496	S497	G597	L577	V578	H580	S581	L582	G583	E584	V585	A586	C587	G588	Y589	A590	D591	Q596	A599	V600	R606	T610	K611	L615	M620	A621	A622	V623
A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494	I495	R496	S497	G597	L577	V578	H580	S581	L582	G583	E584	V585	A586	C587	G588	Y589	A590	D591	Q596	A599	V600	R606	T610	K611	L615	M620	A621	A622	V623
A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494	I495	R496	S497	G597	L577	V578	H580	S581	L582	G583	E584	V585	A586	C587	G588	Y589	A590	D591	Q596	A599	V600	R606	T610	K611	L615	M620	A621	A622	V623
A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494	I495	R496	S497	G597	L577	V578	H580	S581	L582	G583	E584	V585	A586	C587	G588	Y589	A590	D591	Q596	A599	V600	R606	T610	K611	L615	M620	A621	A622	V623
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A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494	I495	R496	S497	G597	L577	V578	H580	S581	L582	G583	E584	V585	A586	C587	G588	Y589	A590	D591	Q596	A599	V600	R606	T610	K611	L615	M620	A621	A622	V623
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A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494	I495	R496	S497	G597	L577	V578	H580	S581	L582	G583	E584	V585	A586	C587	G588	Y589	A590	D591	Q596	A599	V600	R606	T610	K611	L615	M620	A621	A622	V623
A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494	I495	R496	S497	G597	L577	V578	H580	S581	L582	G583	E584	V585	A586	C587	G588	Y589	A590	D591	Q596	A599	V600	R606	T610	K611	L615	M620	A621	A622	V623
A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494	I495	R496	S497	G597	L577	V578	H580	S581	L582	G583	E584	V585	A586	C587	G588	Y589	A590	D591	Q596	A599	V600	R606	T610	K611	L615	M620	A621	A622	V623
A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494	I495	R496	S497	G597	L577	V578	H580	S581	L582	G583	E584	V585	A586	C587	G588	Y589	A590	D591	Q596	A599	V600	R606	T610	K611	L615	M620	A621	A622	V623
A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494	I495	R496	S497	G597	L577	V578	H580	S581	L582	G583	E584	V585	A586	C587	G588	Y589	A590	D591	Q596	A599	V600	R606	T610	K611	L615	M620	A621	A622	V623
A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494	I495	R496	S497	G597	L577	V578	H580	S581	L582	G583	E584	V585	A586	C587	G588	Y589	A590	D591	Q596	A599	V600	R606	T610	K611	L615	M620	A621	A622	V623
A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494	I495	R496	S497	G597	L577	V578	H580	S581	L582	G583	E584	V585	A586	C587	G588	Y589	A590	D591	Q596	A599	V600	R606	T610	K611	L615	M620	A621	A622	V623
A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494	I495	R496	S497	G597	L577	V578	H580	S581	L582	G583	E584	V585	A586	C587	G588	Y589	A590	D591	Q596	A599	V600	R606	T610	K611	L615	M620	A621	A622	V623
A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494	I495	R496	S497	G597	L577	V578	H580	S581	L582	G583	E584	V585	A586	C587	G588	Y589	A590	D591	Q596	A599	V600	R606	T610	K611	L615	M620	A621	A622	V623
A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494	I495	R496	S497	G597	L577	V578	H580	S581	L582	G583	E584	V585	A586	C587	G588	Y589	A590	D591	Q596	A599	V600	R606	T610	K611	L615	M620	A621	A622	V623
A691	P692	P693	L694	L695	E696	E699	C630	K631	G632	A635	R468	Q560	G469	Y470	R477	L563	I564	D565	L566	L567	S568	C569	M570	L492	W493	F494</																													

[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	130804	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	0.750	Depositor
Minimum map value	-0.182	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.028	Depositor
Recommended contour level	0.171	Depositor
Map size (Å)	384.84, 384.84, 384.84	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	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	0.15	0/16198	0.32	6/22023 (0.0%)
1	B	0.19	0/16222	0.34	1/22055 (0.0%)
All	All	0.17	0/32420	0.33	7/44078 (0.0%)

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1195	GLN	N-CA-C	-9.62	100.87	111.36
1	A	1197	GLU	N-CA-C	6.86	118.75	111.28
1	A	979	PRO	N-CA-C	-6.29	104.79	113.53
1	A	237	SER	N-CA-C	6.08	117.57	111.07
1	B	1814	VAL	N-CA-C	-5.75	104.73	111.00

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	9349	15809	532	0
1	B	15857	9380	15826	510	0
2	A	96	52	52	23	0
2	B	96	52	52	11	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	31882	18833	31739	1027	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 16.

The worst 5 of 1027 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:661:PHE:CE2	1:B:665:LEU:HD11	1.80	1.15
1:A:1140:LEU:HD13	1:A:1174:SER:OG	1.50	1.11
1:A:1973:VAL:HB	2:A:2602:NDP:H3D	1.36	1.07
1:A:628:GLU:HA	1:A:631:LYS:HE2	1.33	1.05
1:A:619:ALA:HA	1:A:677:THR:HG21	1.36	1.03

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%)	2014 (98%)	46 (2%)	0	100	100
1	B	2063/2553 (81%)	2018 (98%)	45 (2%)	0	100	100
All	All	4123/5106 (81%)	4032 (98%)	91 (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%)	1699 (100%)	6 (0%)	84	84
1	B	1708/2117 (81%)	1698 (99%)	10 (1%)	78	81
All	All	3413/4234 (81%)	3397 (100%)	16 (0%)	78	83

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1802	GLU
1	B	1801	ASN
1	B	717	ILE
1	B	1371	ILE
1	B	378	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 63 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	2028	ASN
1	B	1595	GLN
1	B	293	HIS
1	B	1447	ASN
1	B	1835	GLN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	2601	-	51,52,52	0.52	0	71,80,80	0.69	1 (1%)
2	NDP	A	2601	-	51,52,52	0.54	0	71,80,80	0.65	1 (1%)
2	NDP	A	2602	-	51,52,52	0.50	0	71,80,80	0.77	2 (2%)
2	NDP	B	2602	-	51,52,52	0.49	0	71,80,80	0.77	2 (2%)

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	2601	-	-	13/34/77/77	0/5/5/5
2	NDP	A	2601	-	-	10/34/77/77	0/5/5/5
2	NDP	A	2602	-	-	9/34/77/77	0/5/5/5
2	NDP	B	2602	-	-	10/34/77/77	0/5/5/5

There are no bond length outliers.

The worst 5 of 6 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2602	NDP	P2B-O2B-C2B	-4.14	112.38	123.43
2	B	2602	NDP	P2B-O2B-C2B	-3.93	112.94	123.43
2	B	2601	NDP	P2B-O2B-C2B	-3.63	113.75	123.43
2	B	2602	NDP	C3N-C2N-N1N	-2.71	119.23	123.20
2	A	2602	NDP	C3N-C2N-N1N	-2.14	120.06	123.20

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

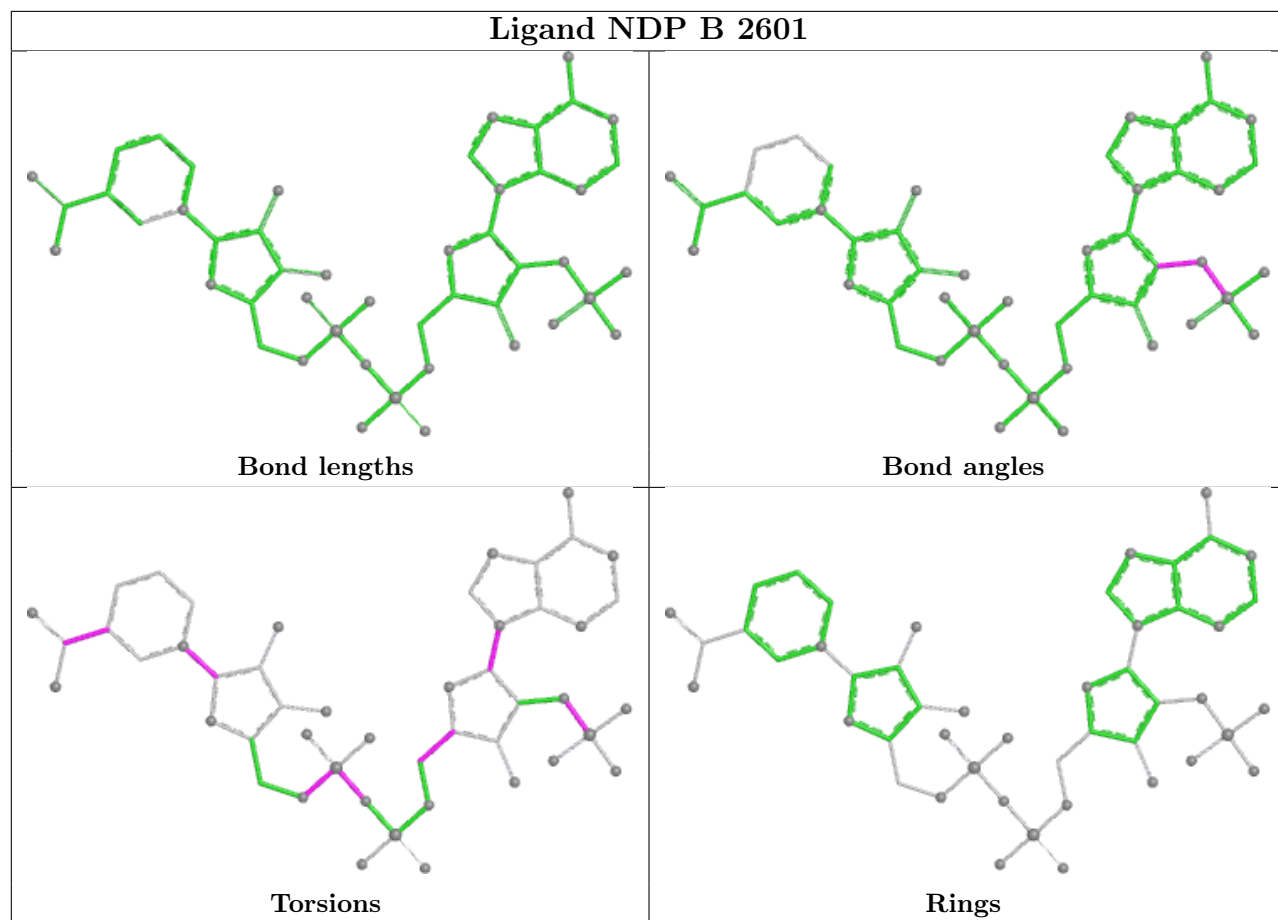
Mol	Chain	Res	Type	Atoms
2	A	2601	NDP	C5D-O5D-PN-O3
2	A	2601	NDP	C5D-O5D-PN-O1N
2	A	2601	NDP	O4D-C1D-N1N-C2N
2	A	2601	NDP	C2N-C3N-C7N-N7N
2	A	2602	NDP	C3B-C4B-C5B-O5B

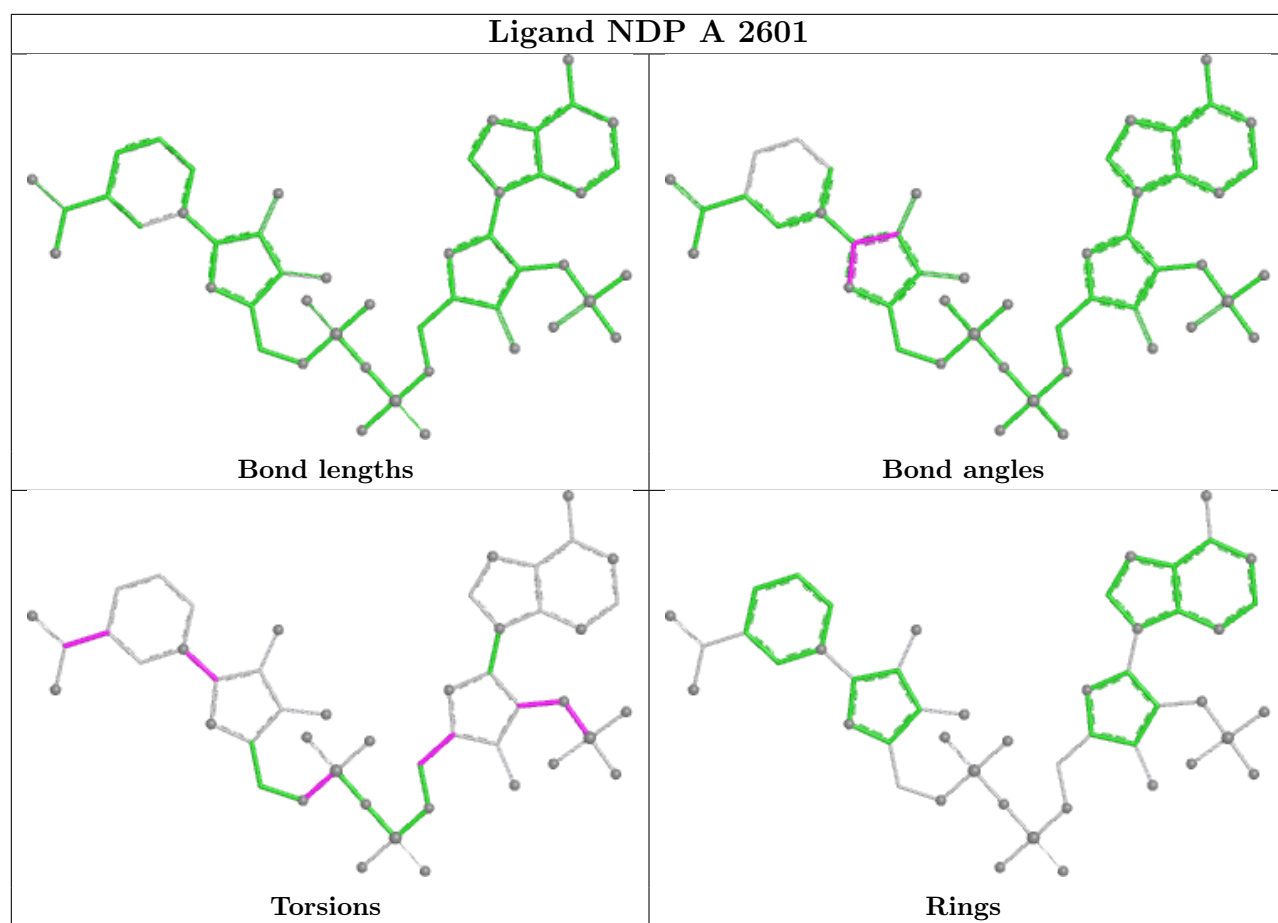
There are no ring outliers.

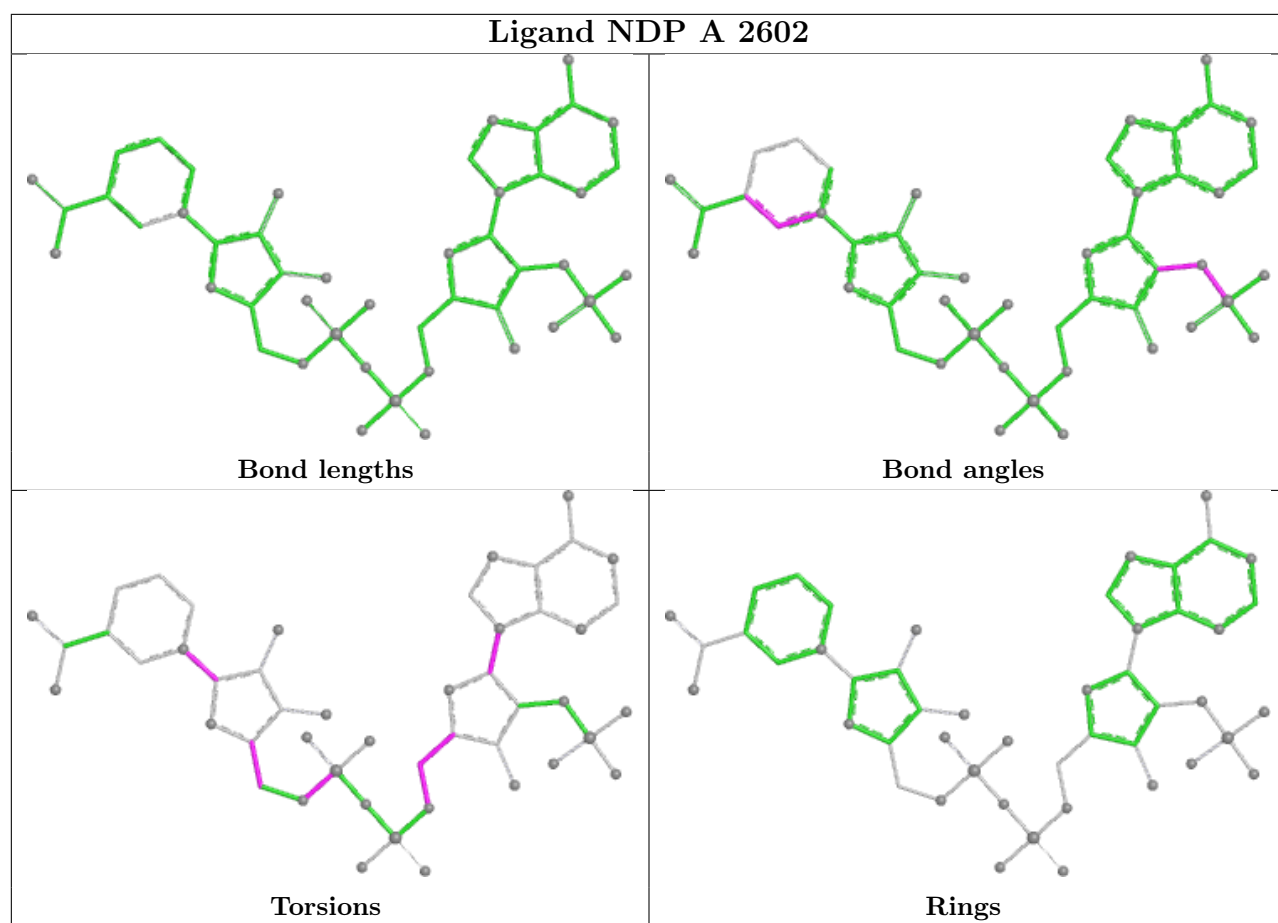
4 monomers are involved in 34 short contacts:

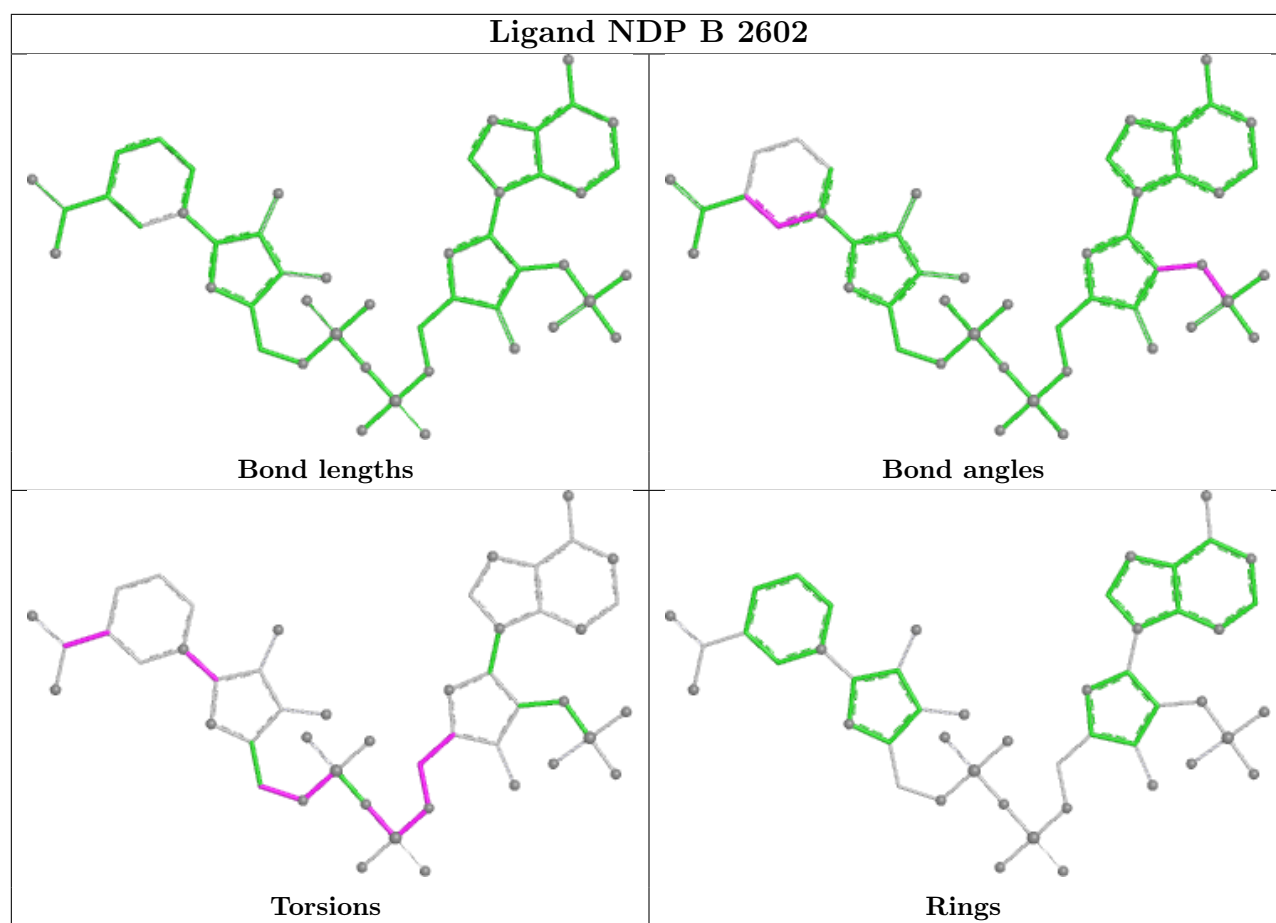
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2601	NDP	2	0
2	A	2601	NDP	3	0
2	A	2602	NDP	20	0
2	B	2602	NDP	9	0

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.

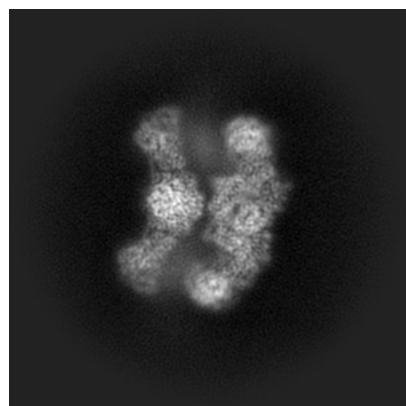
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43337. These allow visual inspection of the internal detail of the map and identification of artifacts.

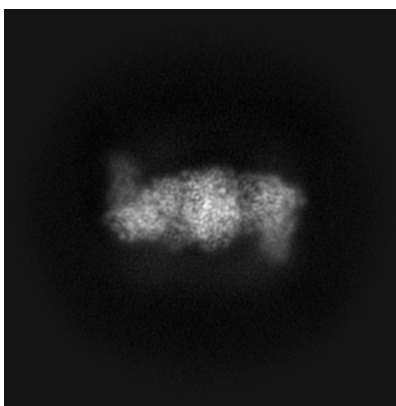
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

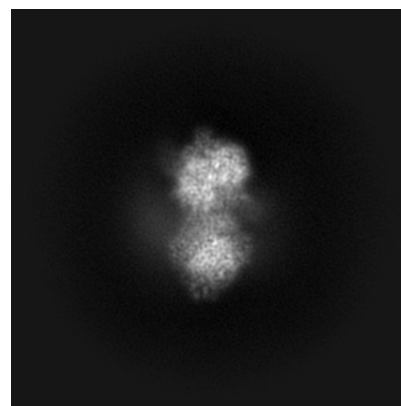
6.1.1 Primary map



X

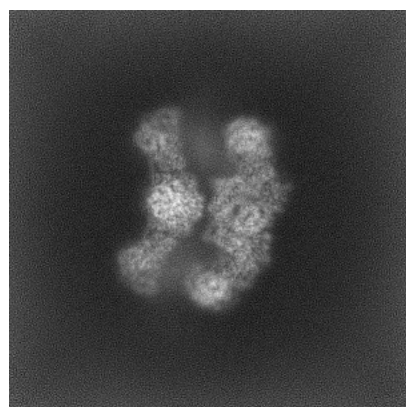


Y

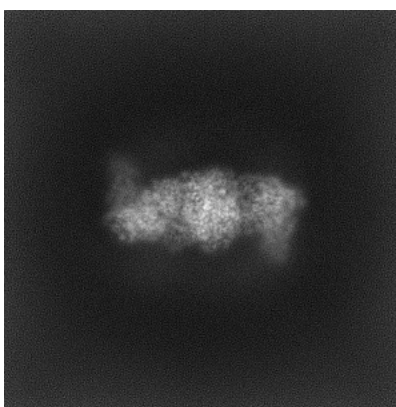


Z

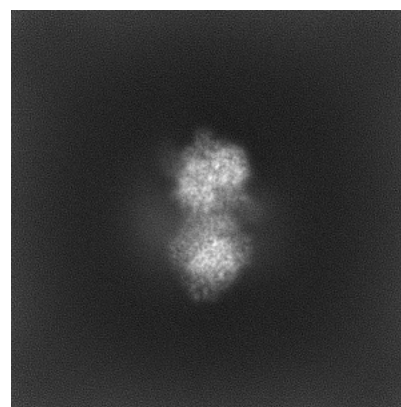
6.1.2 Raw map



X



Y

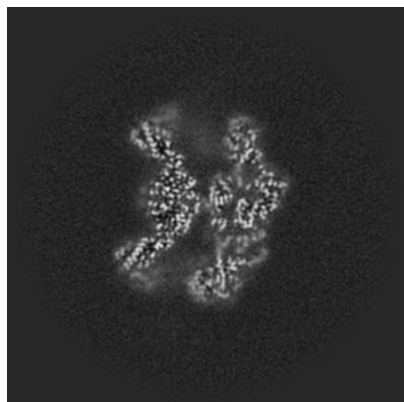


Z

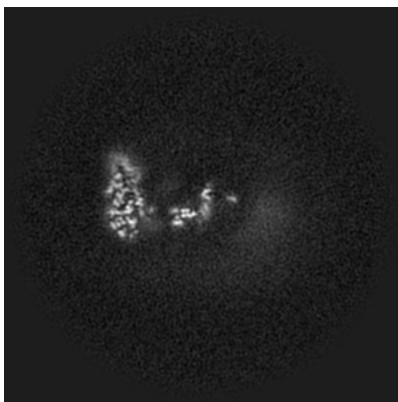
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

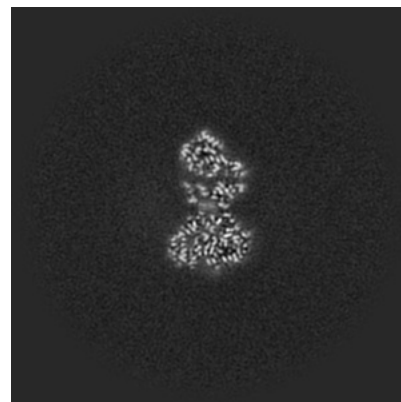
6.2.1 Primary map



X Index: 180

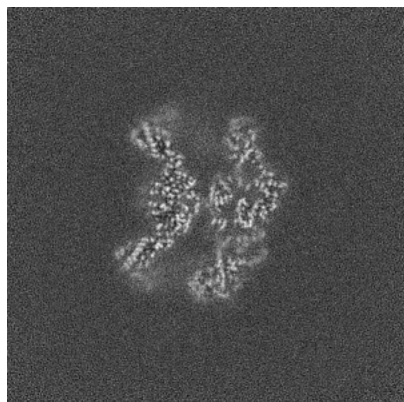


Y Index: 180

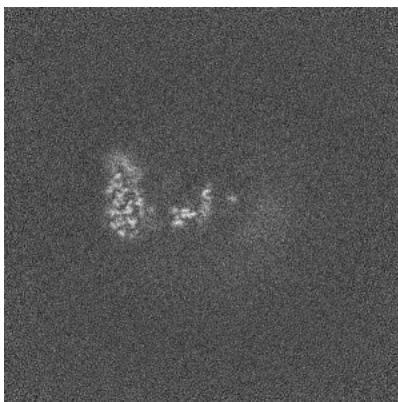


Z Index: 180

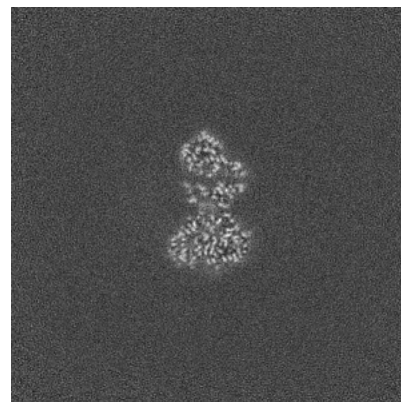
6.2.2 Raw map



X Index: 180



Y Index: 180

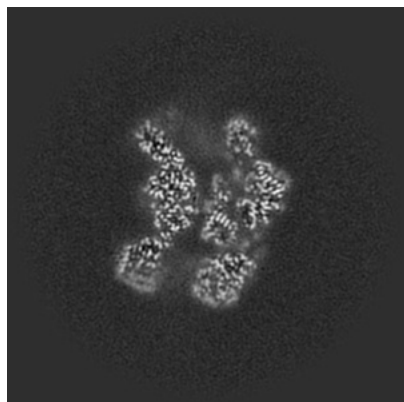


Z Index: 180

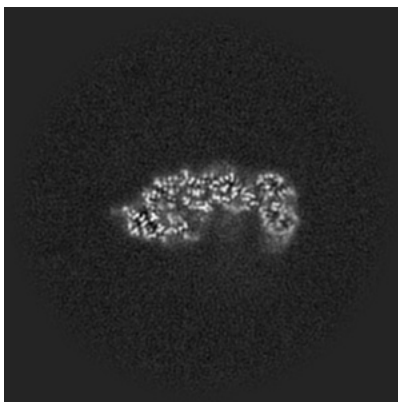
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

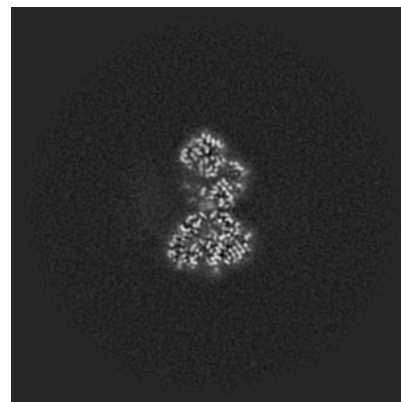
6.3.1 Primary map



X Index: 176

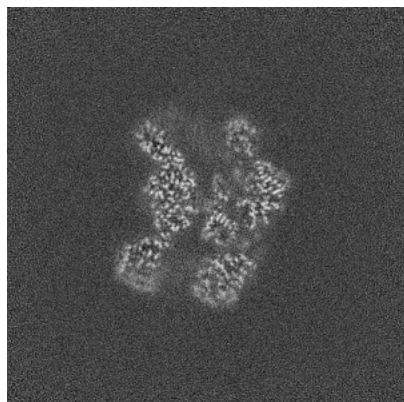


Y Index: 208

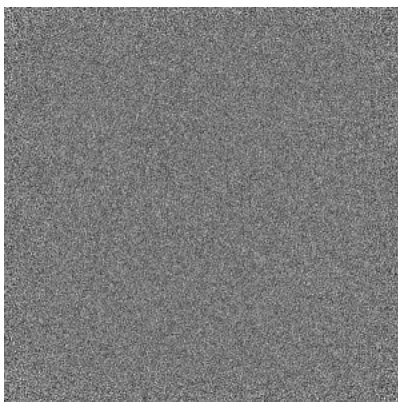


Z Index: 182

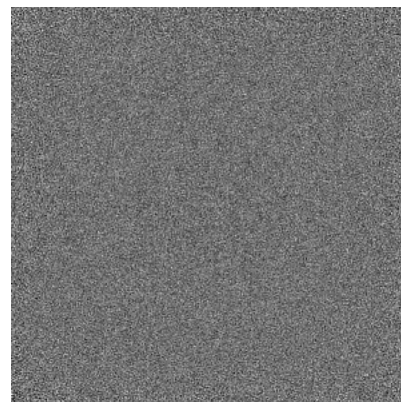
6.3.2 Raw map



X Index: 176



Y Index: 0



Z Index: 359

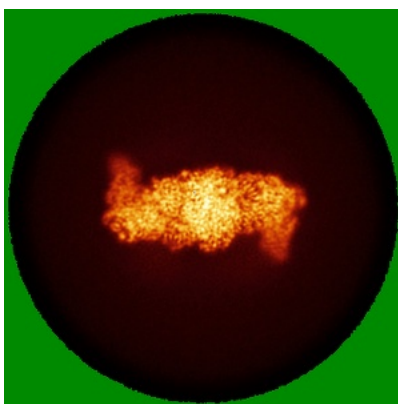
The images above show the largest variance slices of the map in three orthogonal directions.

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

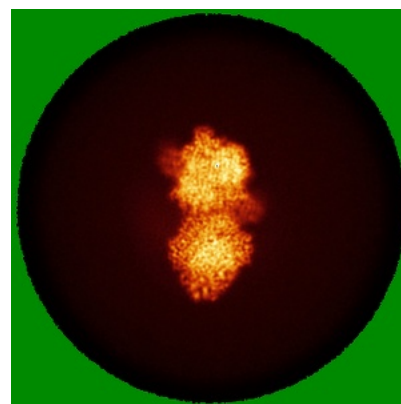
6.4.1 Primary map



X

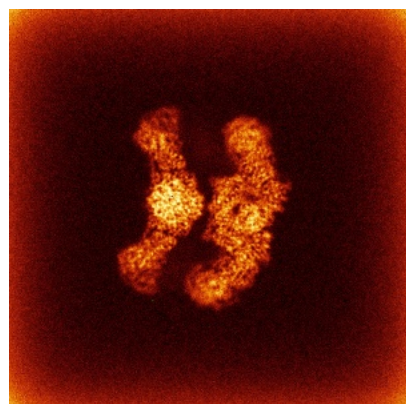


Y

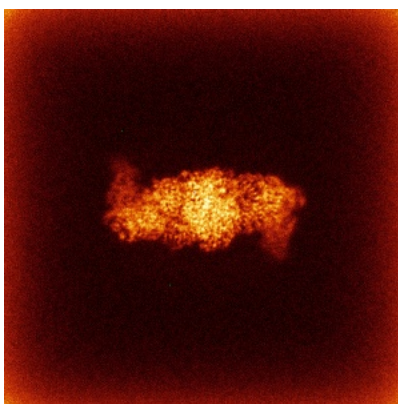


Z

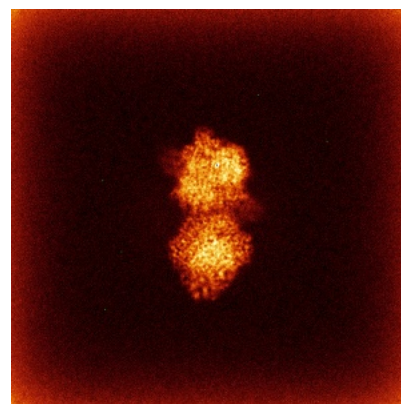
6.4.2 Raw map



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](#)

This section was not generated.

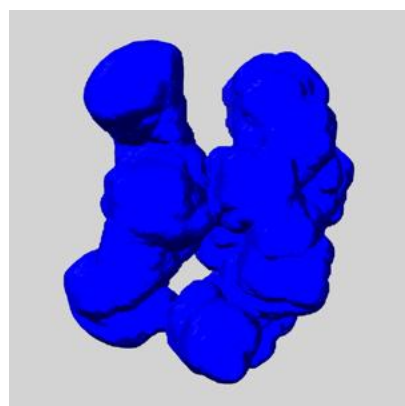
6.6 Mask visualisation [i](#)

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

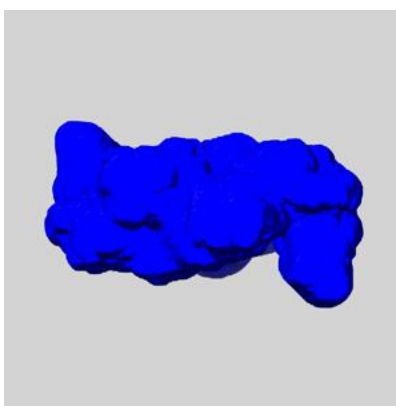
A mask typically either:

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

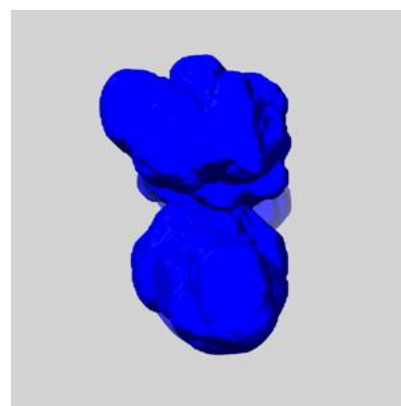
6.6.1 emd_43337_msk_1.map [i](#)



X



Y

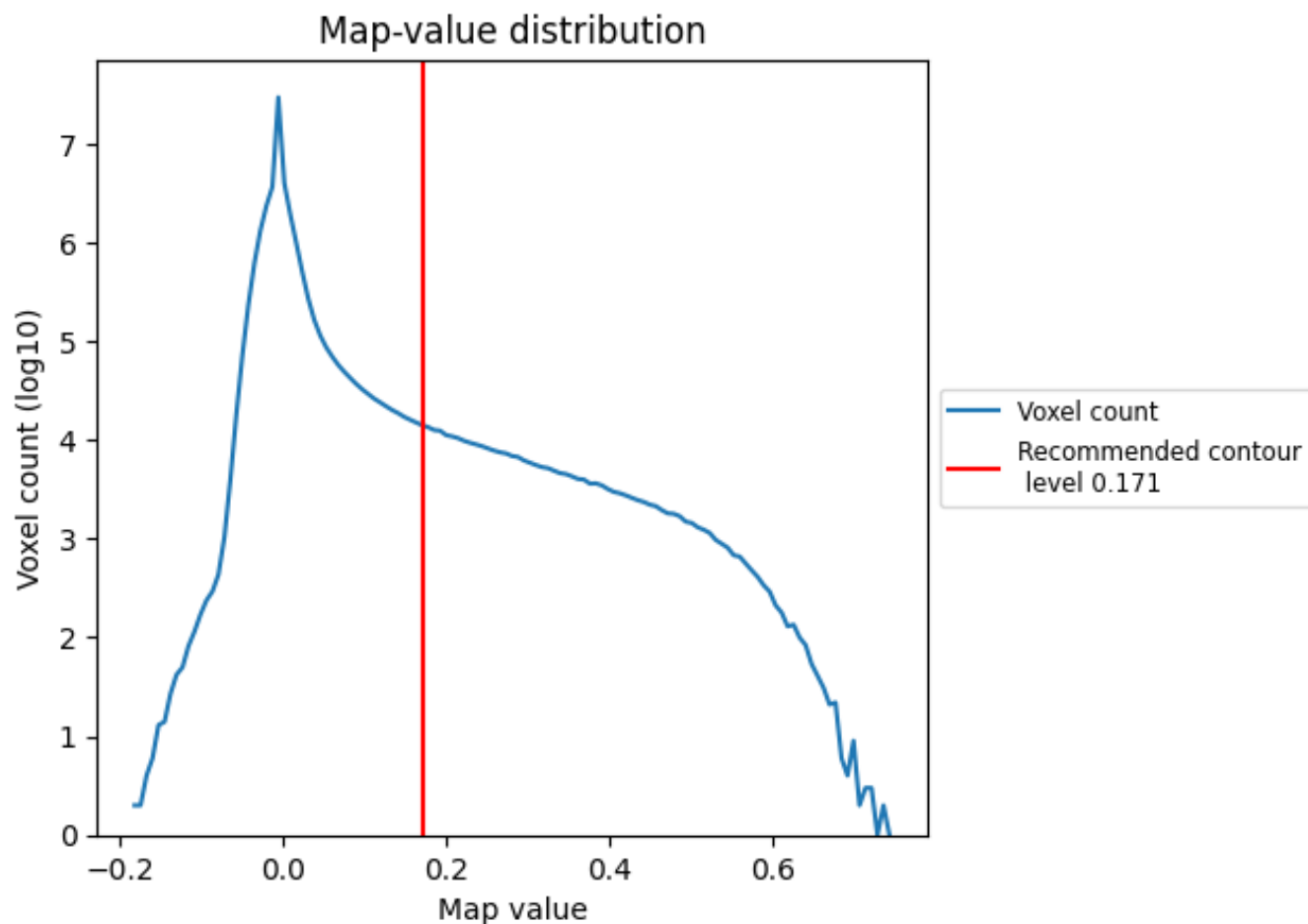


Z

7 Map analysis [i](#)

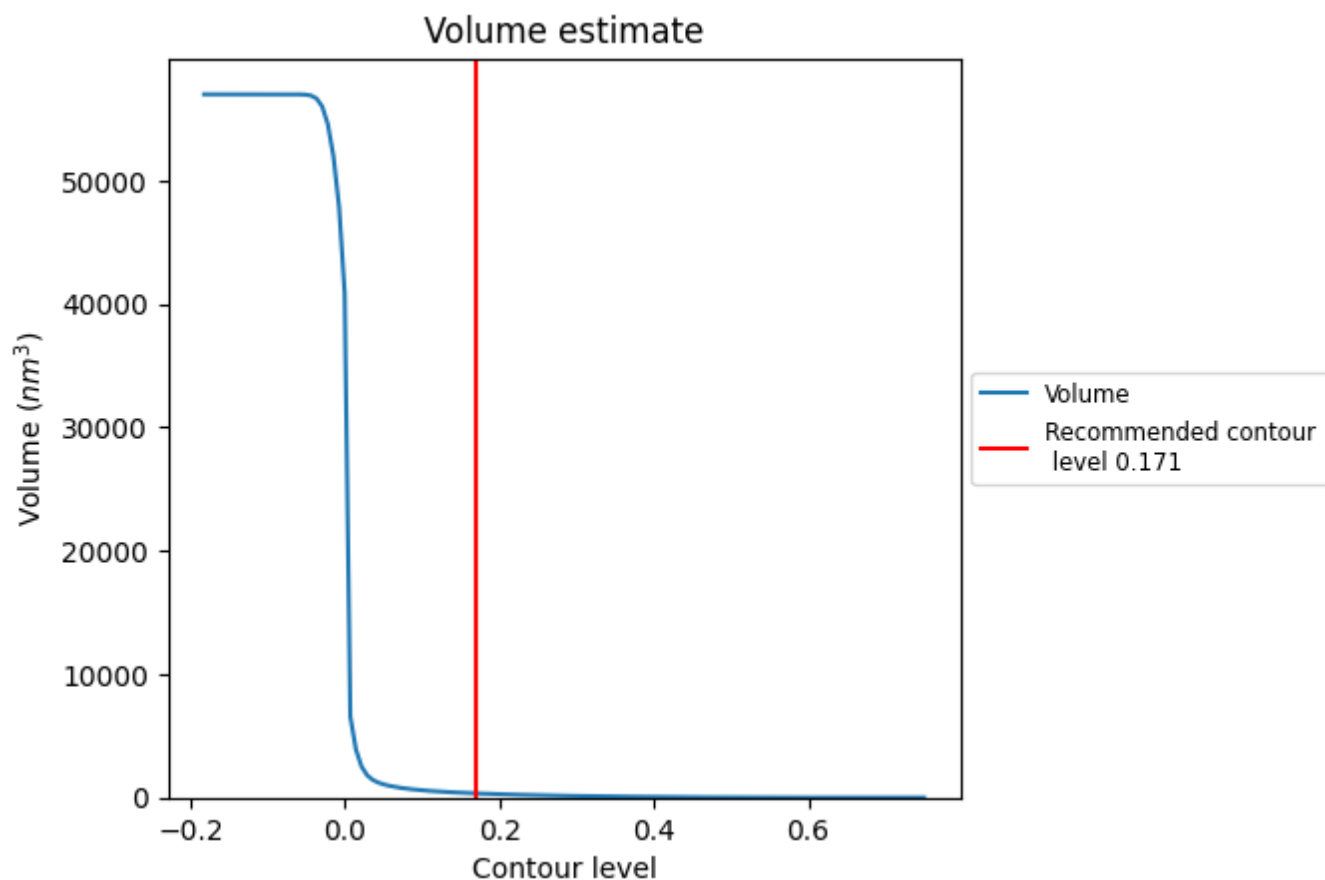
This section contains the results of statistical analysis of the map.

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.

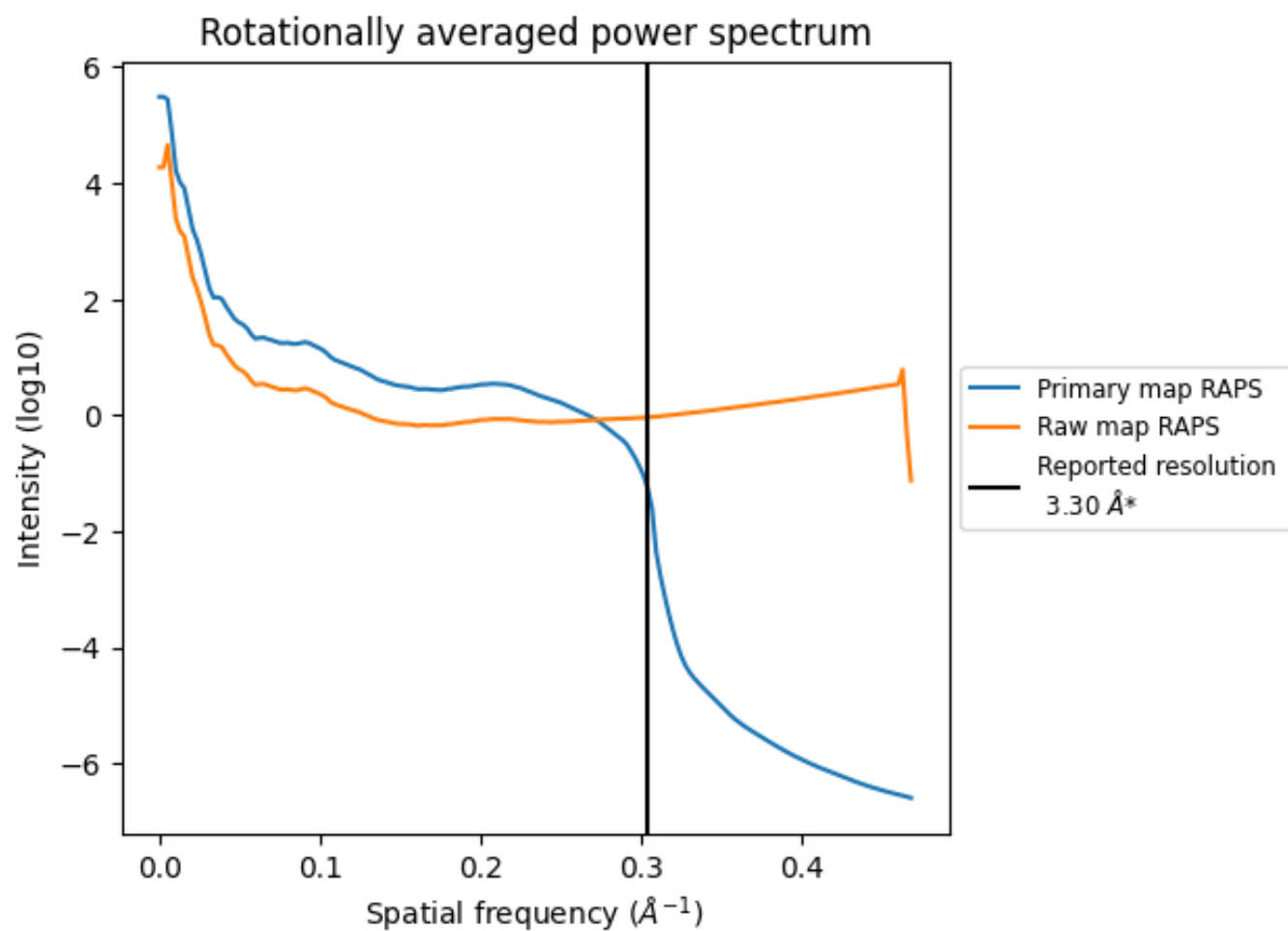
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 336 nm³; this corresponds to an approximate mass of 304 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 ⓘ

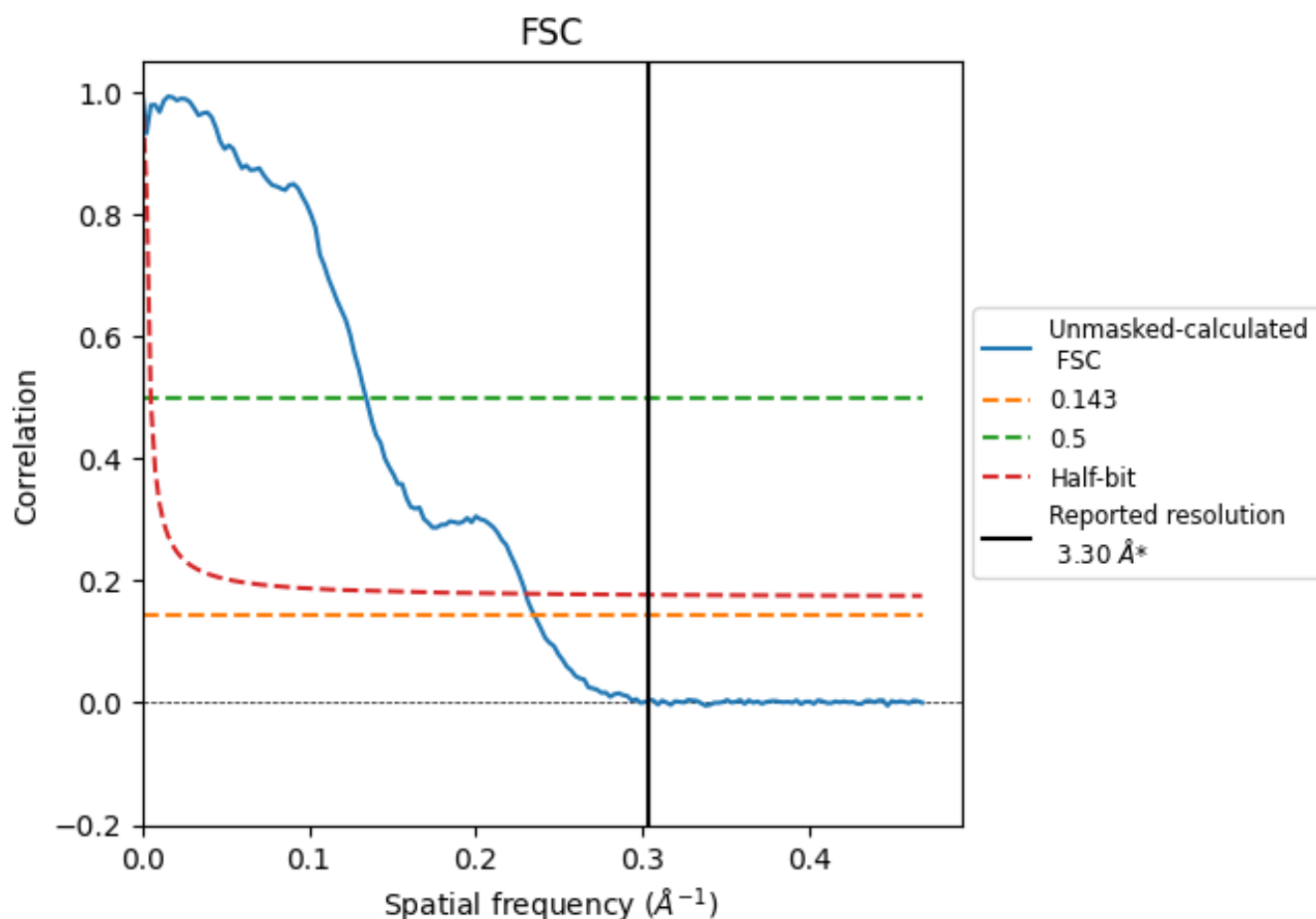


*Reported resolution corresponds to spatial frequency of 0.303 $\text{\AA}^{-1}$

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⁻¹

8.2 Resolution estimates [i](#)

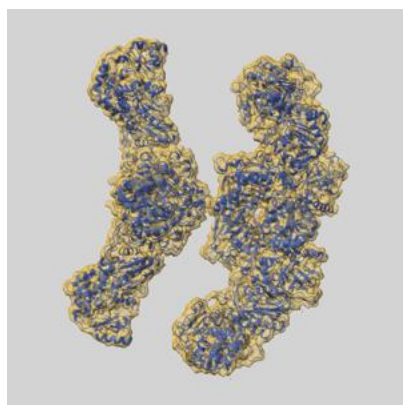
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.25	7.46	4.35

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

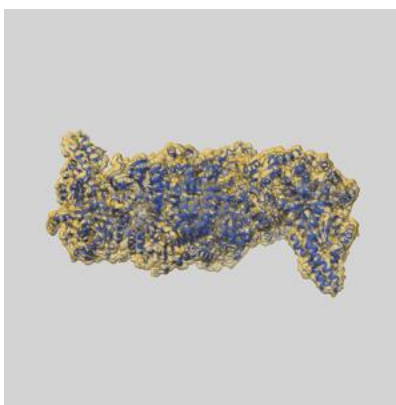
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43337 and PDB model 8VLE. Per-residue inclusion information can be found in section 3 on page 7.

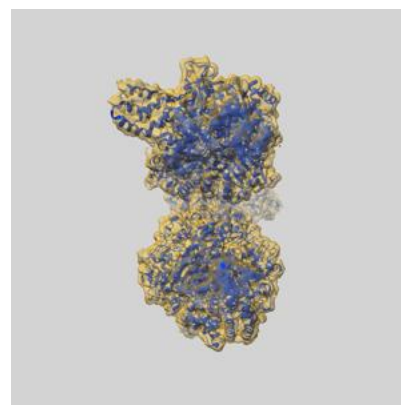
9.1 Map-model overlay [i](#)



X



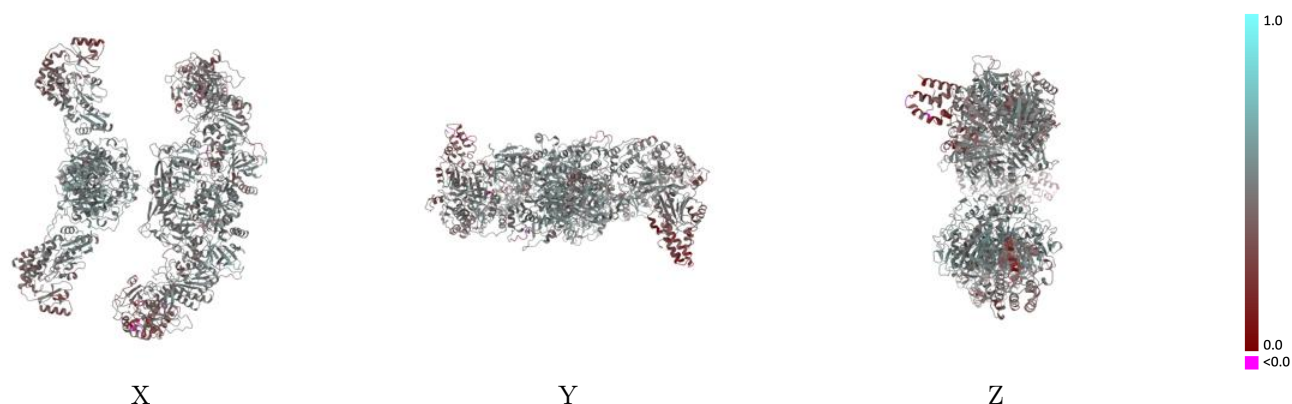
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.171 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](#)

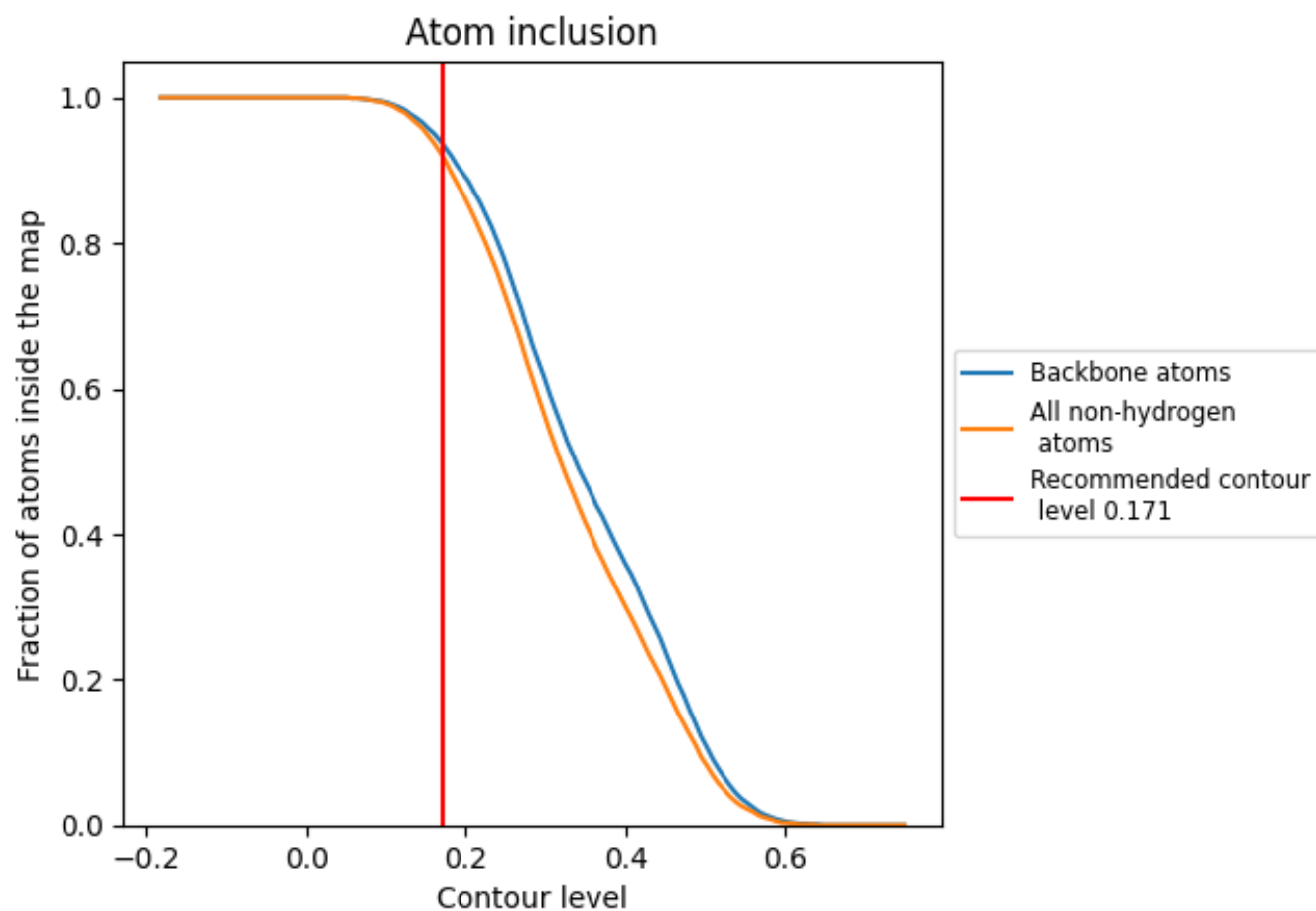


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

This section was not generated.

9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 92% 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 (0.171) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9200	0.4690
A	0.9220	0.4710
B	0.9160	0.4670

