



# wwPDB EM Validation Summary Report ⓘ

Mar 8, 2026 – 01:37 AM UTC

PDB ID : 8VMC / pdb\_00008vmc  
EMDB ID : EMD-43355  
Title : Composite structure of human FASN with NADPH in State 6  
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>.

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

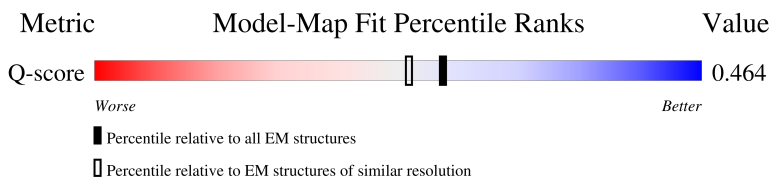
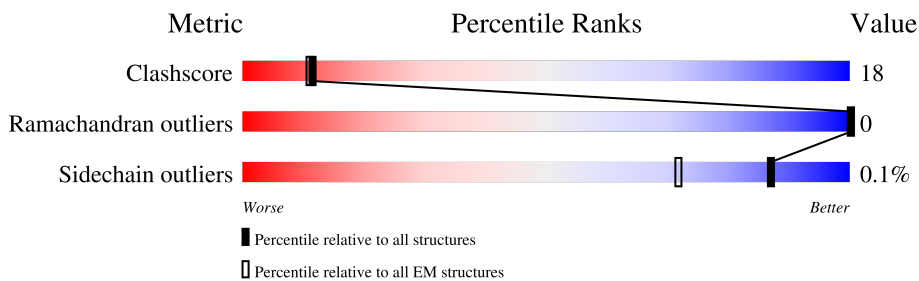
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01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

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  $\geq 3$ , 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	<p>57% 24% 19%</p>
1	B	2553	<p>59% 22% 19%</p>

## 2 Entry composition i

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	25176	10041	9343	2785	2934	73	0	0
1	B	2071	25237	10054	9380	2789	2941	73	0	0

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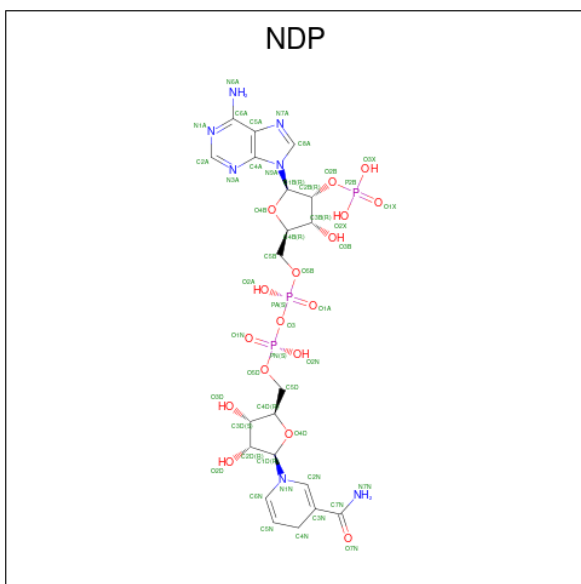
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP P49327
A	-4	MET	-	expression tag	UNP P49327
A	-3	GLY	-	expression tag	UNP P49327
A	-2	SER	-	expression tag	UNP P49327
A	-1	GLY	-	expression tag	UNP P49327
A	0	ILE	-	expression tag	UNP P49327
A	1	PRO	-	expression tag	UNP P49327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

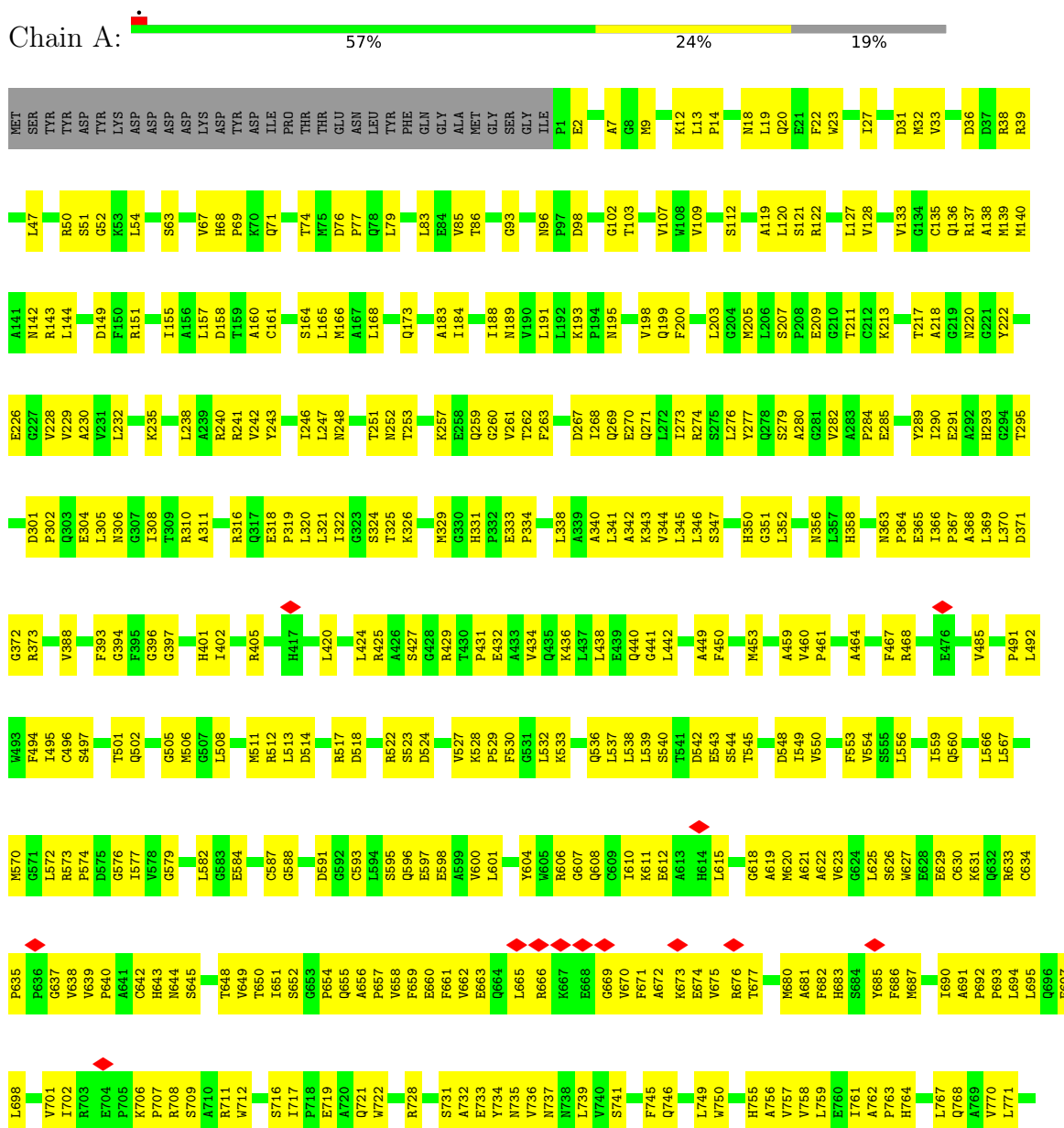


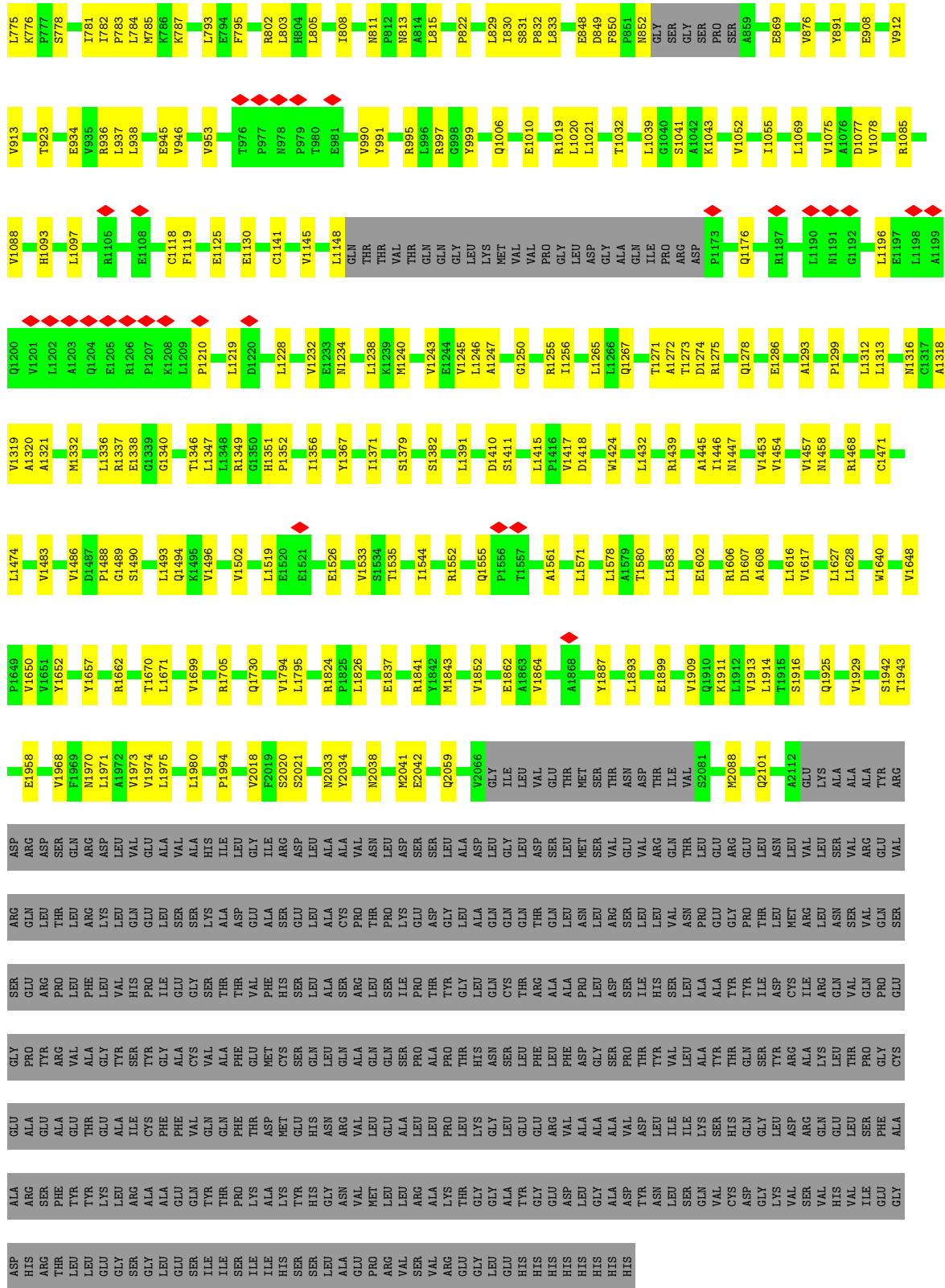
Mol	Chain	Residues	Atoms					AltConf	
			Total	C	H	N	O		P
2	A	1	74	21	26	7	17	3	0
2	A	1	74	21	26	7	17	3	0
2	B	1	74	21	26	7	17	3	0
2	B	1	74	21	26	7	17	3	0

### 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



Q1374	Q1204	A1102	R652	L759	P693	V550	E476	P367	A283	L206	P124	R38	MET
V1377	E1205	V1111	GLY	E760	L694	H551	R477	A368	F284	L207	L127	R39	SER
R1387	R1206	T1120	GLY	I761	L695	V554		L369	E285	P208	L128	L47	TYR
L1208	P1207	E1126	GLY	A765	Q696	S555	Q483	D371	T290	E209	Y130	R50	ASP
L1389	L1208	L1128	GLY	L766	E697	L556	Q484	G372	G210	G210	G131	K63	LYS
G1390	PRO	G1126	PRO	L767	L698	T557	V485	R373	E291	T211	M132		ASP
L1391	SER	L1128	SER	Q768	K699	I561	E489	L374	H293	C212	V133		ASP
K1392	A959	L1129	GLY	A769	K700	G662	R490	V376	G294	A214	C135	D56	ASP
Y1396	D865	S1129	GLY	V770	I702	L563	R490	V376	T295	F215	C135	L57	ASP
F1401	S870	E1130	GLY	K772	R703	L566	L492		V299	D216	A138	S58	LYS
V1417	D881	C1141	GLY	G774	E704	L567	W493		P302	T217	M139	R59	ASP
V1424	L775	V1145	GLY	K776	K706	L587	F494		F393			F60	TYR
K1429	L783	L1150	THR	I781	W112	L577	I495		Q303	G221	M142	P69	ASP
D1436	P783	THR	THR	P783	L713	I577	C996		G303	G222	M143	P69	ILE
A1445	L784	VAL	THR	I784	S714	S581	E304		L305	Y222	R143	K70	PRO
I1446	W935	GLN	GLN	M785	P718	L582	L305		N306	R224	L144	Q71	THR
V1457	R936	GLY	GLY	K786	E719	L582	G498		G307	R223	F150	H73	THR
C1471	L937	LEU	LEU	K787	A720	E584	M499		I308	G227	A156	R80	GLU
L1474	E939	LYS	LYS	H788	Q721	E584	M499		I308	G227	A156	R80	GLU
E1485	A940	MET	MET	H789	Q721	E584	M499		I308	G227	A156	R80	GLU
V1486	S941	VAL	VAL	R790	W722	V585	M500		I308	G227	A156	R80	GLU
L1493	E948	VAL	VAL	N792	S724	V585	M500		I308	G227	A156	R80	GLU
L1497	N949	PRO	PRO	F795	S725	G588	M506		I308	G227	A156	R80	GLU
Q1498	L976	GLY	GLY	L803	E727	G588	M506		I308	G227	A156	R80	GLU
L1501	P977	ASP	ASP	H804	R729	G588	M506		I308	G227	A156	R80	GLU
R1515	H978	ALA	ALA	L805	S730	G588	M506		I308	G227	A156	R80	GLU
F1517	E981	ILE	ILE	A810	E731	G588	M506		I308	G227	A156	R80	GLU
E1521	P982	PRO	PRO	M811	A732	G588	M506		I308	G227	A156	R80	GLU
R1552	R997	ARG	ARG	A814	E732	G588	M506		I308	G227	A156	R80	GLU
Q1555	E1014	ASP	ASP	P817	E732	G588	M506		I308	G227	A156	R80	GLU
S1570	K1043	ASP	ASP	F821	E732	G588	M506		I308	G227	A156	R80	GLU
I1588	L1046	ILE	ILE	P822	E732	G588	M506		I308	G227	A156	R80	GLU
Q1595	L1071	PRO	PRO	A823	E732	G588	M506		I308	G227	A156	R80	GLU
D1596	D1072	PRO	PRO	F743	E732	G588	M506		I308	G227	A156	R80	GLU
E1602	L1072	PRO	PRO	L744	E732	G588	M506		I308	G227	A156	R80	GLU
	D1077	PRO	PRO	F745	E732	G588	M506		I308	G227	A156	R80	GLU
	V1078	PRO	PRO	V746	E732	G588	M506		I308	G227	A156	R80	GLU
	V1079	PRO	PRO	L747	E732	G588	M506		I308	G227	A156	R80	GLU
	V1080	PRO	PRO	L748	E732	G588	M506		I308	G227	A156	R80	GLU
	T1087	PRO	PRO	L749	E732	G588	M506		I308	G227	A156	R80	GLU
	V1088	PRO	PRO	L750	E732	G588	M506		I308	G227	A156	R80	GLU
	V1089	PRO	PRO	L751	E732	G588	M506		I308	G227	A156	R80	GLU
	L1198	PRO	PRO	L752	E732	G588	M506		I308	G227	A156	R80	GLU
	L1371	PRO	PRO	L753	E732	G588	M506		I308	G227	A156	R80	GLU
	L1372	PRO	PRO	L754	E732	G588	M506		I308	G227	A156	R80	GLU
	S1373	PRO	PRO	L755	E732	G588	M506		I308	G227	A156	R80	GLU
	L1202	PRO	PRO	L756	E732	G588	M506		I308	G227	A156	R80	GLU
	A1203	PRO	PRO	L757	E732	G588	M506		I308	G227	A156	R80	GLU
				L758	E732	G588	M506		I308	G227	A156	R80	GLU
				L759	E732	G588	M506		I308	G227	A156	R80	GLU
				L760	E732	G588	M506		I308	G227	A156	R80	GLU
				L761	E732	G588	M506		I308	G227	A156	R80	GLU
				L762	E732	G588	M506		I308	G227	A156	R80	GLU
				L763	E732	G588	M506		I308	G227	A156	R80	GLU
				L764	E732	G588	M506		I308	G227	A156	R80	GLU
				L765	E732	G588	M506		I308	G227	A156	R80	GLU
				L766	E732	G588	M506		I308	G227	A156	R80	GLU
				L767	E732	G588	M506		I308	G227	A156	R80	GLU
				L768	E732	G588	M506		I308	G227	A156	R80	GLU
				L769	E732	G588	M506		I308	G227	A156	R80	GLU
				L770	E732	G588	M506		I308	G227	A156	R80	GLU
				L771	E732	G588	M506		I308	G227	A156	R80	GLU
				L772	E732	G588	M506		I308	G227	A156	R80	GLU
				L773	E732	G588	M506		I308	G227	A156	R80	GLU
				L774	E732	G588	M506		I308	G227	A156	R80	GLU
				L775	E732	G588	M506		I308	G227	A156	R80	GLU
				L776	E732	G588	M506		I308	G227	A156	R80	GLU
				L777	E732	G588	M506		I308	G227	A156	R80	GLU
				L778	E732	G588	M506		I308	G227	A156	R80	GLU
				L779	E732	G588	M506		I308	G227	A156	R80	GLU
				L780	E732	G588	M506		I308	G227	A156	R80	GLU
				L781	E732	G588	M506		I308	G227	A156	R80	GLU
				L782	E732	G588	M506		I308	G227	A156	R80	GLU
				L783	E732	G588	M506		I308	G227	A156	R80	GLU
				L784	E732	G588	M506		I308	G227	A156	R80	GLU
				L785	E732	G588	M506		I308	G227	A156	R80	GLU
				L786	E732	G588	M506		I308	G227	A156	R80	GLU
				L787	E732	G588	M506		I308	G227	A156	R80	GLU
				L788	E732	G588	M506		I308	G227	A156	R80	GLU
				L789	E732	G588	M506		I308	G227	A156	R80	GLU
				L790	E732	G588	M506		I308	G227	A156	R80	GLU
				L791	E732	G588	M506		I308	G227	A156	R80	GLU
				L792	E732	G588	M506		I308	G227	A156	R80	GLU
				L793	E732	G588	M506		I308	G227	A156	R80	GLU
				L794	E732	G588	M506		I308	G227	A156	R80	GLU
				L795	E732	G588	M506		I308	G227	A156	R80	GLU
				L796	E732	G588	M506		I308	G227	A156	R80	GLU
				L797	E732	G588	M506		I308	G227	A156	R80	GLU
				L798	E732	G588	M506		I308	G227	A156	R80	GLU
				L799	E732	G588	M506		I308	G227	A156	R80	GLU
				L800	E732	G588	M506		I308	G227	A156	R80	GLU
				L801	E732	G588	M506		I308	G227	A156	R80	GLU
				L802	E732	G588	M506		I308	G227	A156	R80	GLU
				L803	E732	G588	M506		I308	G227	A156	R80	GLU
				L804	E732	G588	M506		I308	G227	A156	R80	GLU
				L805	E732	G588	M506		I308	G227	A156	R80	GLU
				L806	E732	G588	M506		I308	G227	A156	R80	GLU
				L807	E732	G588	M506		I308	G227	A156	R80	GLU
				L808	E732	G588	M506		I308	G227	A156	R80	GLU
				L809	E732	G588	M506		I308	G227	A156	R80	GLU
				L810	E732	G588	M506		I308	G227	A156	R80	GLU
				L811	E732	G588	M506		I308	G227	A156	R80	GLU
				L812	E732	G588	M506		I308	G227	A156	R80	GLU
				L813	E732	G588	M506		I308	G227	A156	R80	GLU



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	119577	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	0.790	Depositor
Minimum map value	-0.215	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.173	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 [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	0.16	0/16198	0.25	0/22023
1	B	0.22	0/16222	0.35	2/22055 (0.0%)
All	All	0.19	0/32420	0.31	2/44078 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	783	PRO	CB-CA-C	-6.75	103.13	111.64
1	B	1370	GLY	N-CA-C	-5.49	108.16	114.69

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	554	0
1	B	15857	9380	15826	601	0
2	A	96	52	52	0	0
2	B	96	52	52	3	0
All	All	31882	18827	31739	1133	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 18.

The worst 5 of 1133 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:1369:GLN:HA	1:B:1372:LEU:HD11	1.27	1.15
1:B:322:ILE:HD11	1:B:376:VAL:HG22	1.17	1.14
1:B:1372:LEU:HD22	1:B:1377:TRP:CZ2	1.81	1.14
1:B:1372:LEU:HD22	1:B:1377:TRP:CE2	1.82	1.13
1:A:155:ILE:CG2	1:B:157:LEU:HD22	1.83	1.08

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%)	2004 (97%)	56 (3%)	0	100	100
1	B	2063/2553 (81%)	2003 (97%)	60 (3%)	0	100	100
All	All	4123/5106 (81%)	4007 (97%)	116 (3%)	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%)	1705 (100%)	0	100	100
1	B	1708/2117 (81%)	1705 (100%)	3 (0%)	87	88
All	All	3413/4234 (81%)	3410 (100%)	3 (0%)	87	90

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

Mol	Chain	Res	Type
1	B	277	TYR
1	B	1671	LEU
1	B	1748	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 66 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	1595	GLN
1	B	1731	HIS
1	B	1983	GLN
1	A	1193	ASN
1	A	1110	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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	2602	-	51,52,52	0.52	0	71,80,80	0.67	1 (1%)
2	NDP	B	2601	-	51,52,52	0.48	0	71,80,80	0.78	1 (1%)
2	NDP	A	2601	-	51,52,52	0.50	0	71,80,80	0.75	2 (2%)
2	NDP	B	2602	-	51,52,52	0.52	0	71,80,80	0.66	1 (1%)

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	2602	-	-	13/34/77/77	0/5/5/5
2	NDP	B	2601	-	-	14/34/77/77	0/5/5/5
2	NDP	A	2601	-	-	13/34/77/77	0/5/5/5
2	NDP	B	2602	-	-	12/34/77/77	0/5/5/5

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2601	NDP	P2B-O2B-C2B	-5.03	110.00	123.43
2	B	2602	NDP	P2B-O2B-C2B	-3.74	113.44	123.43
2	A	2602	NDP	P2B-O2B-C2B	-3.41	114.33	123.43
2	A	2601	NDP	O2B-C2B-C3B	2.08	119.13	111.68
2	A	2601	NDP	O3B-C3B-C2B	2.03	116.86	111.19

There are no chirality outliers.

5 of 52 torsion outliers are listed below:

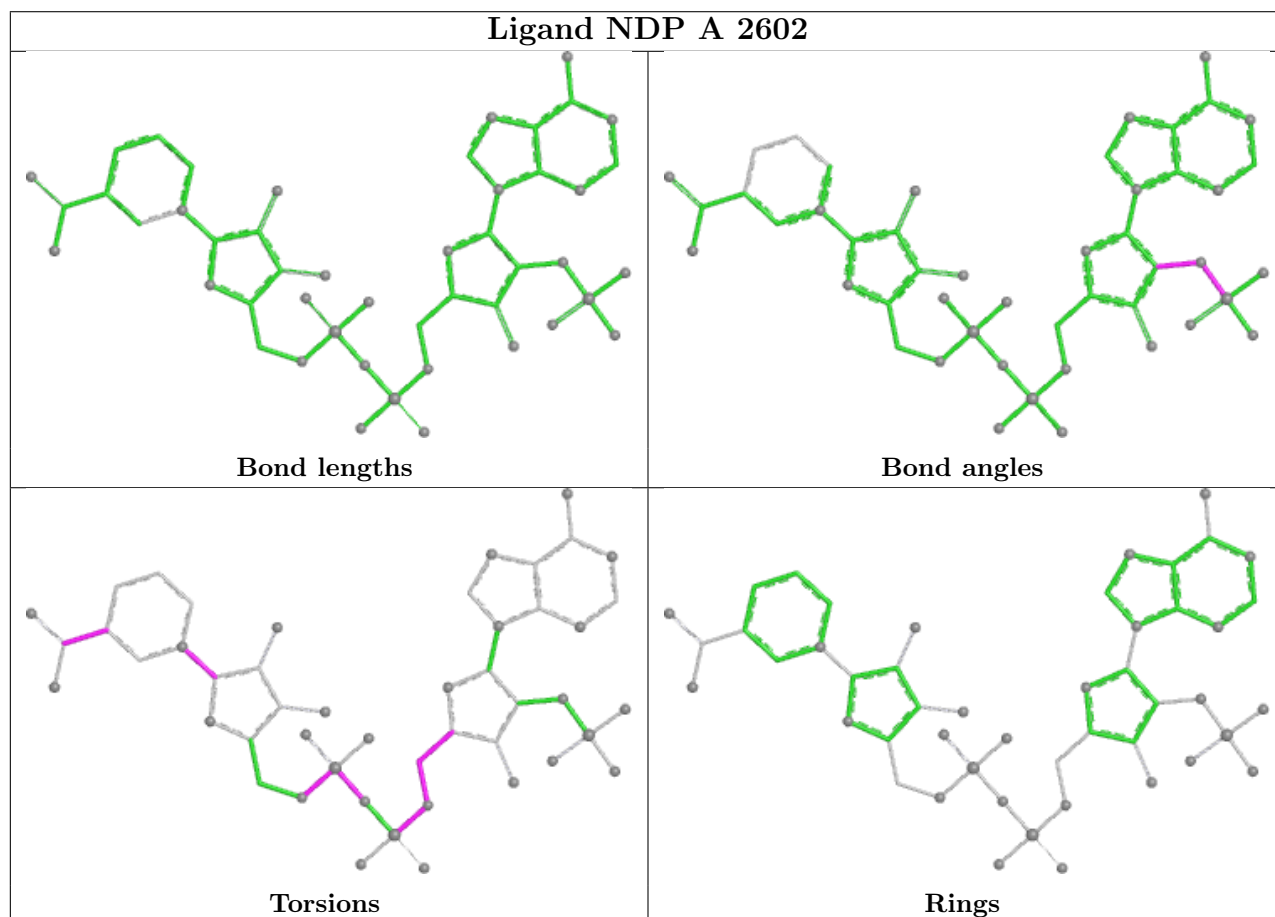
Mol	Chain	Res	Type	Atoms
2	A	2601	NDP	C5D-O5D-PN-O3
2	A	2601	NDP	C5D-O5D-PN-O1N
2	A	2601	NDP	C5D-O5D-PN-O2N
2	A	2601	NDP	O4D-C1D-N1N-C2N
2	A	2601	NDP	C2N-C3N-C7N-O7N

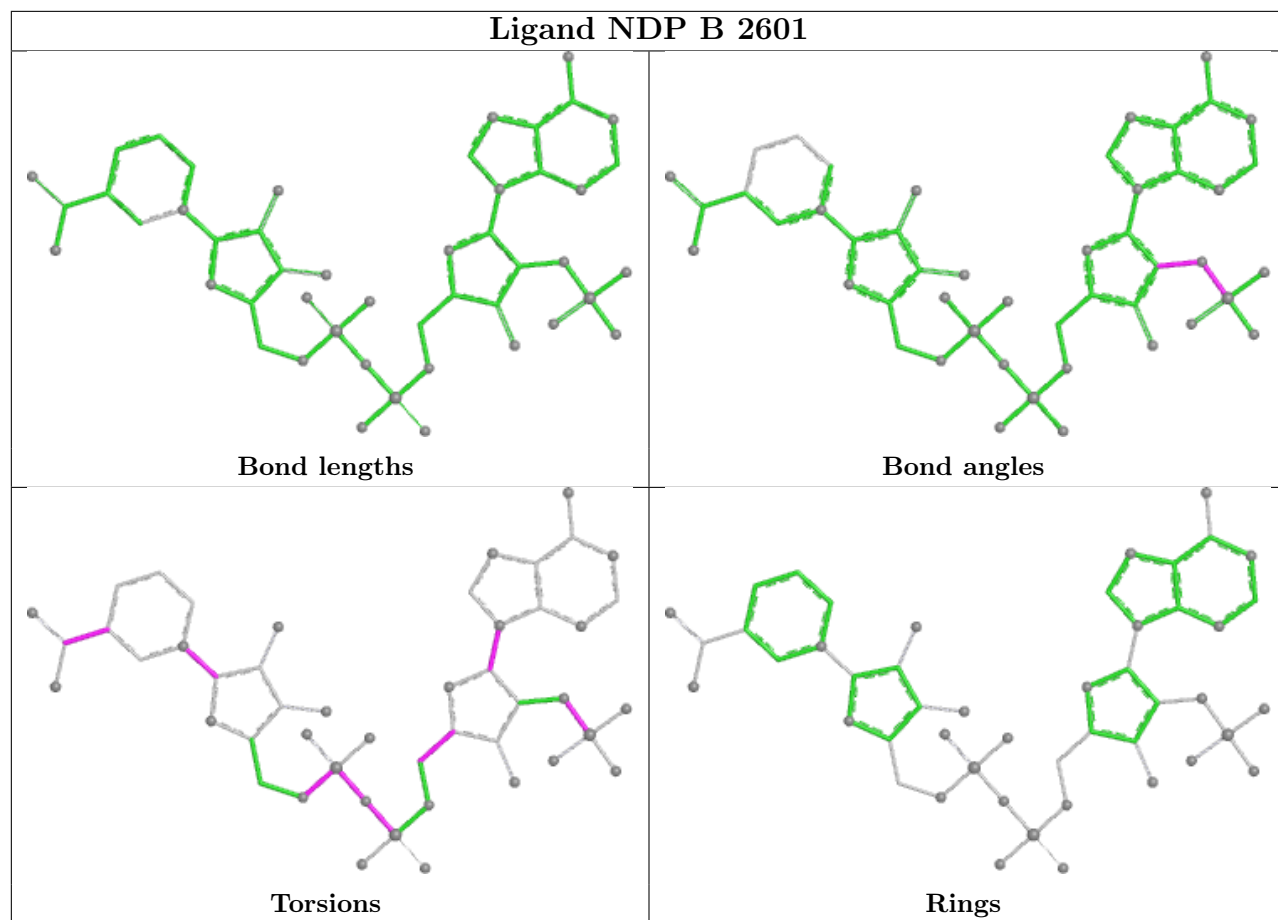
There are no ring outliers.

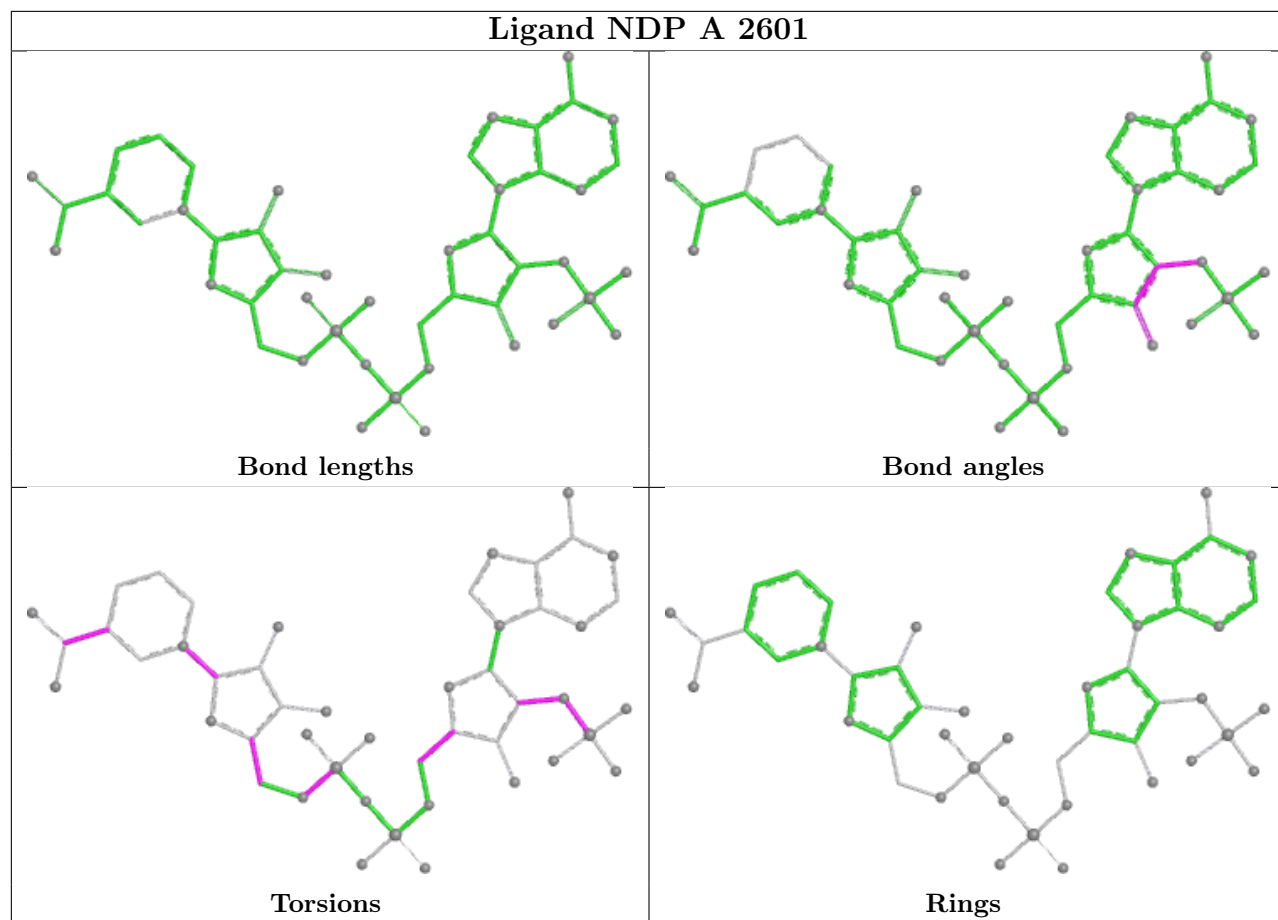
1 monomer is involved in 3 short contacts:

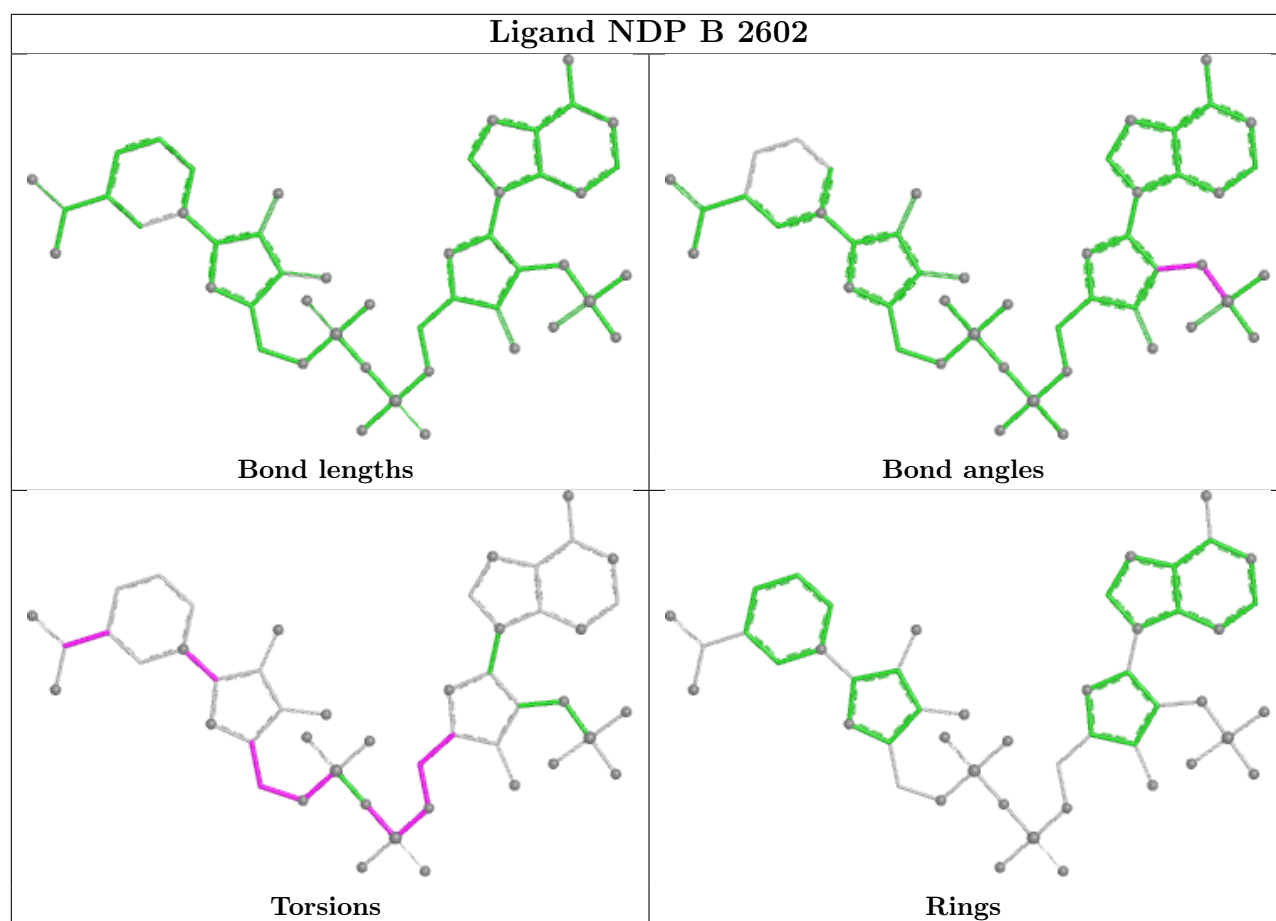
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2602	NDP	3	0

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.

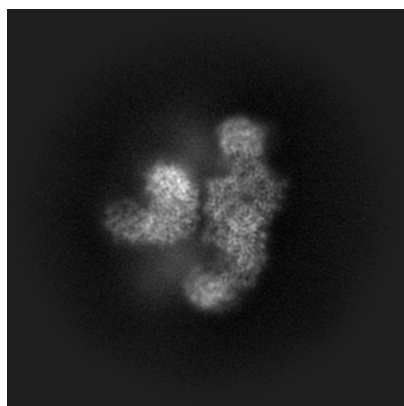
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43355. These allow visual inspection of the internal detail of the map and identification of artifacts.

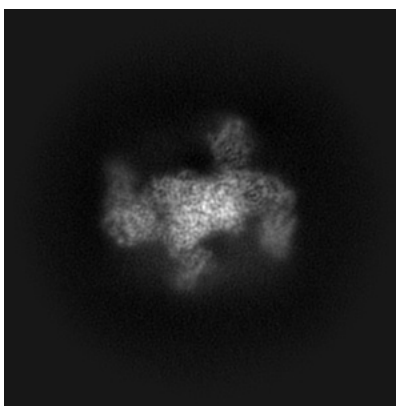
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

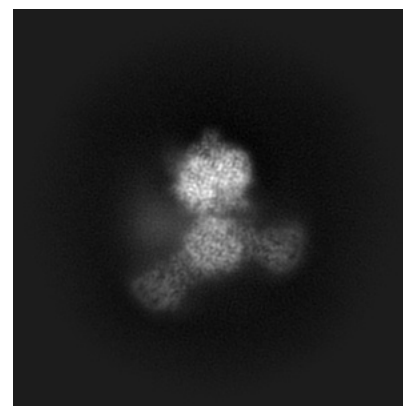
#### 6.1.1 Primary map



X

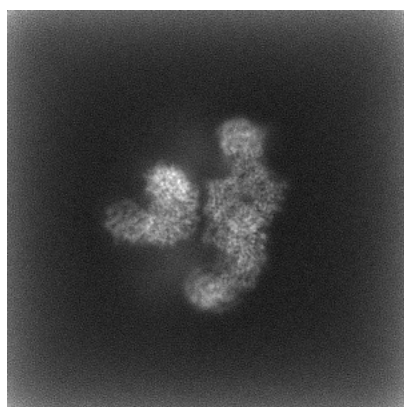


Y

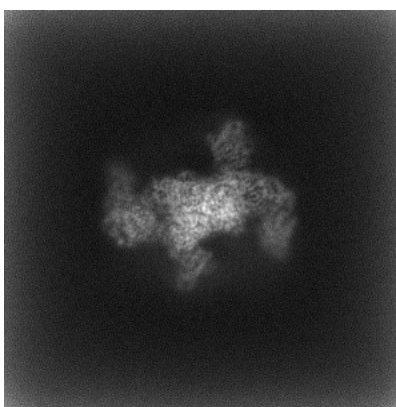


Z

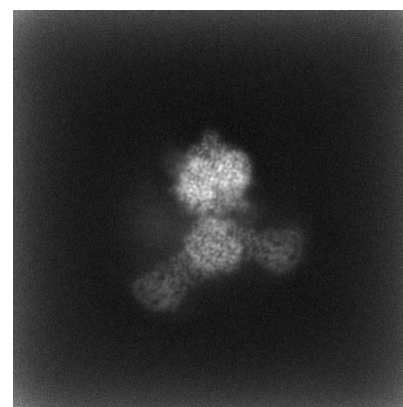
#### 6.1.2 Raw map



X



Y

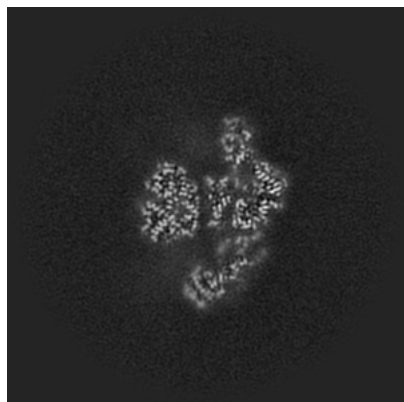


Z

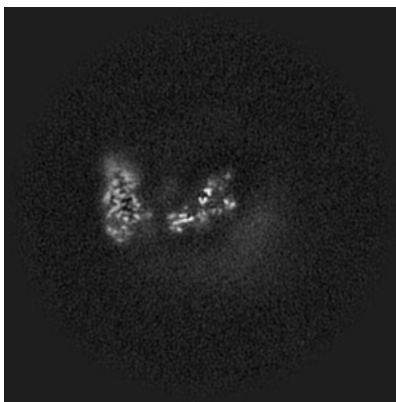
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

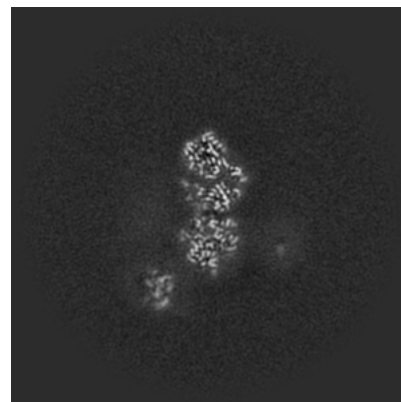
### 6.2.1 Primary map



X Index: 180

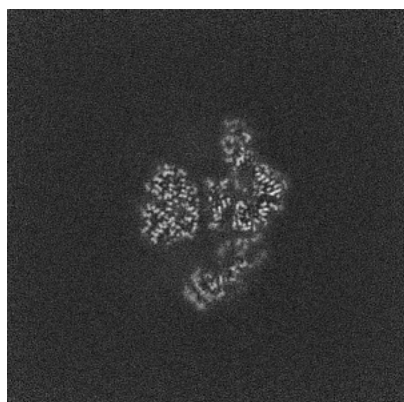


Y Index: 180



Z Index: 180

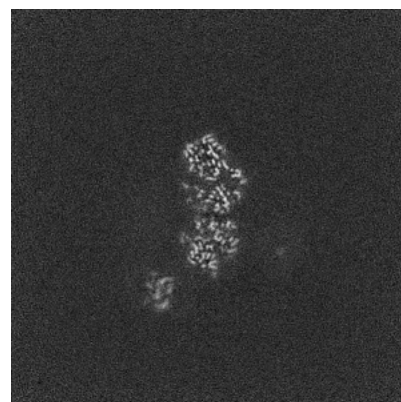
### 6.2.2 Raw map



X Index: 180



Y Index: 180

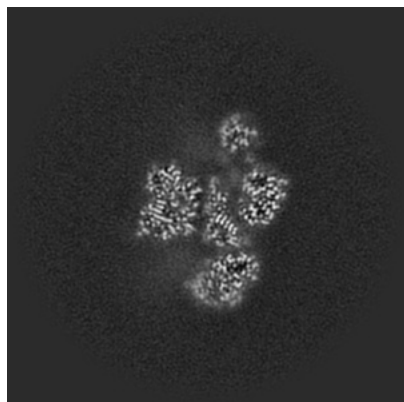


Z Index: 180

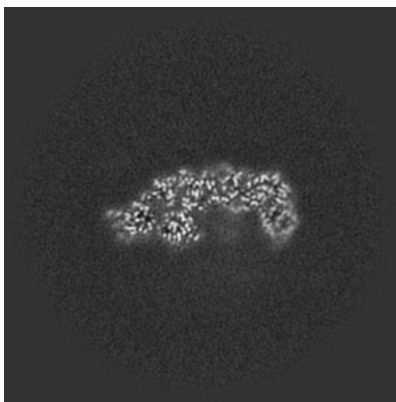
The images above show central slices of the map in three orthogonal directions.

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

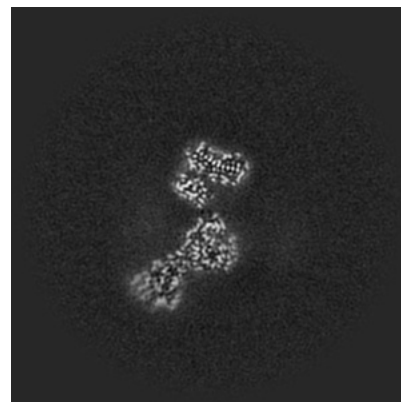
### 6.3.1 Primary map



X Index: 173

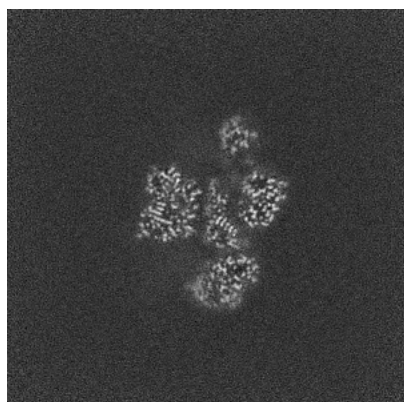


Y Index: 205

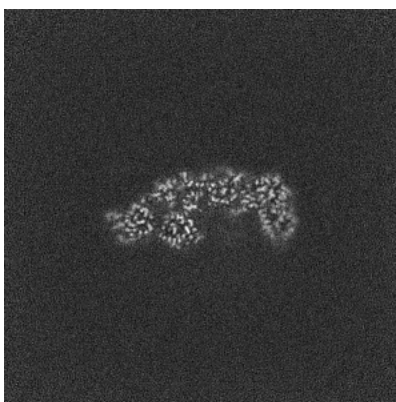


Z Index: 169

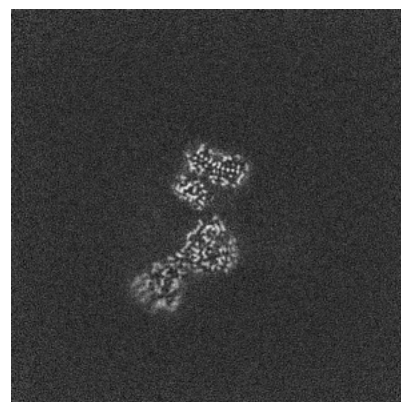
### 6.3.2 Raw map



X Index: 173



Y Index: 204

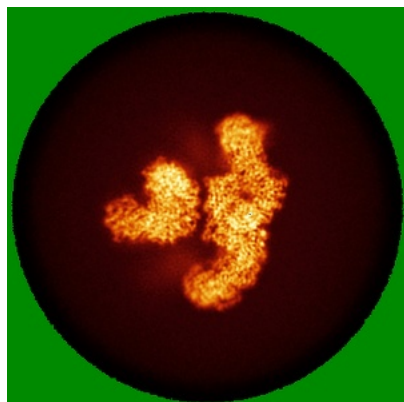


Z Index: 169

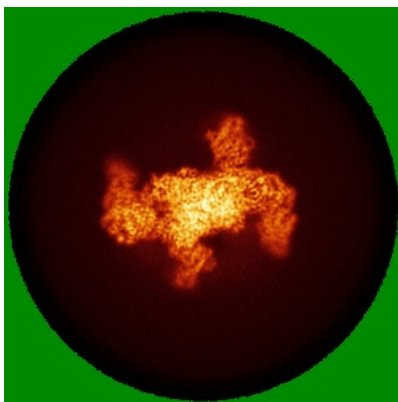
The images above show the largest variance slices of the map in three orthogonal directions.

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

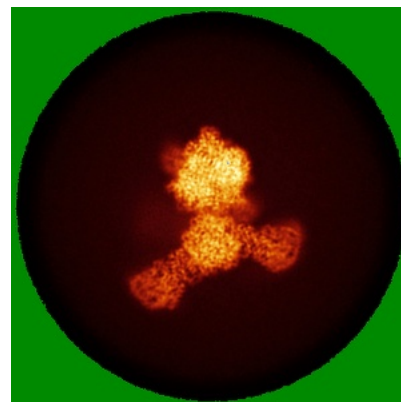
### 6.4.1 Primary map



X

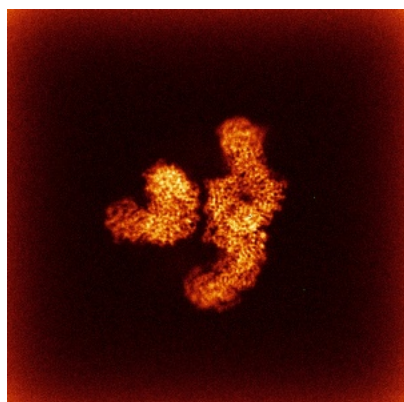


Y

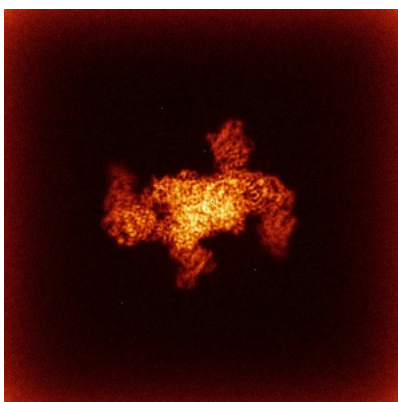


Z

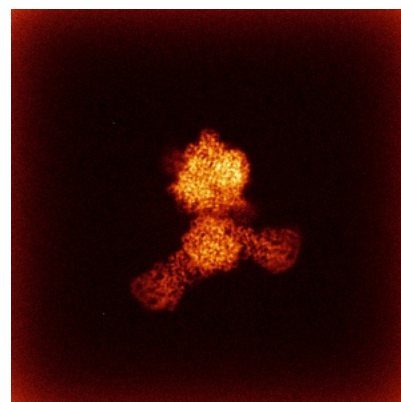
### 6.4.2 Raw map



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.

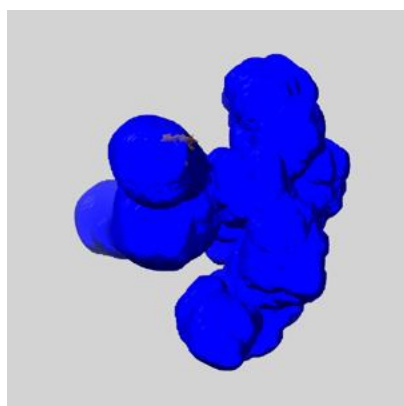
## 6.6 Mask visualisation [i](#)

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

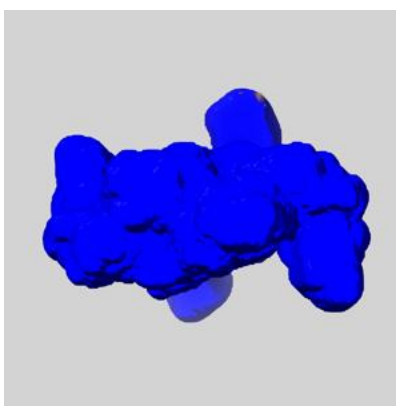
A mask typically either:

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

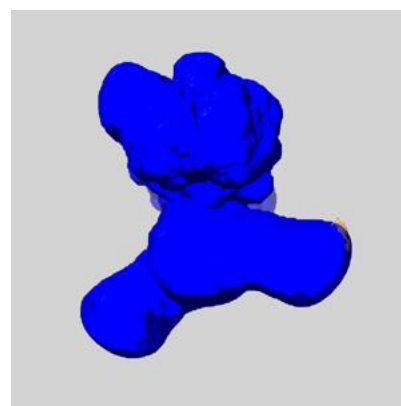
### 6.6.1 emd\_43355\_msk\_1.map [i](#)



X



Y

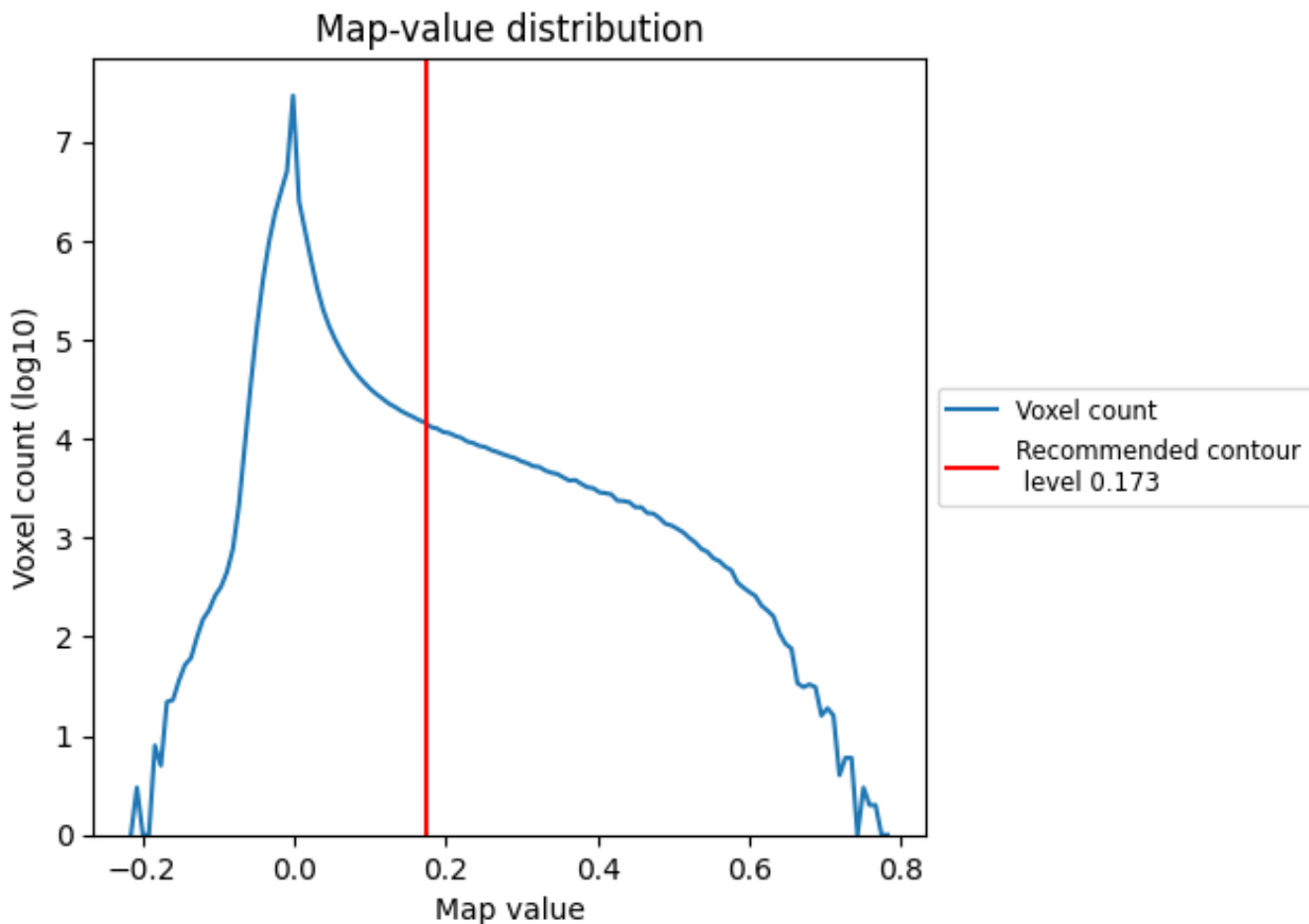


Z

## 7 Map analysis [i](#)

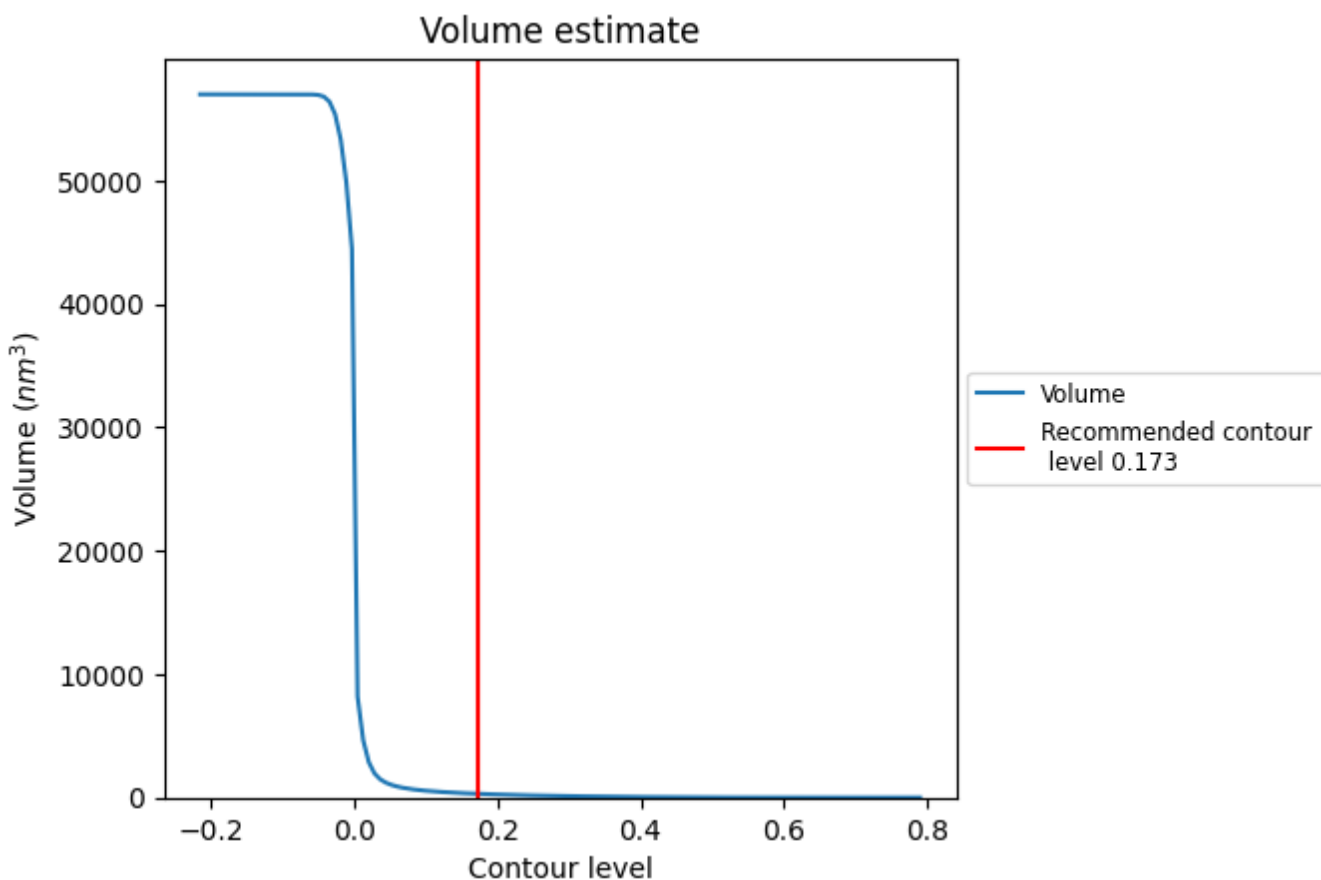
This section contains the results of statistical analysis of the map.

### 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.

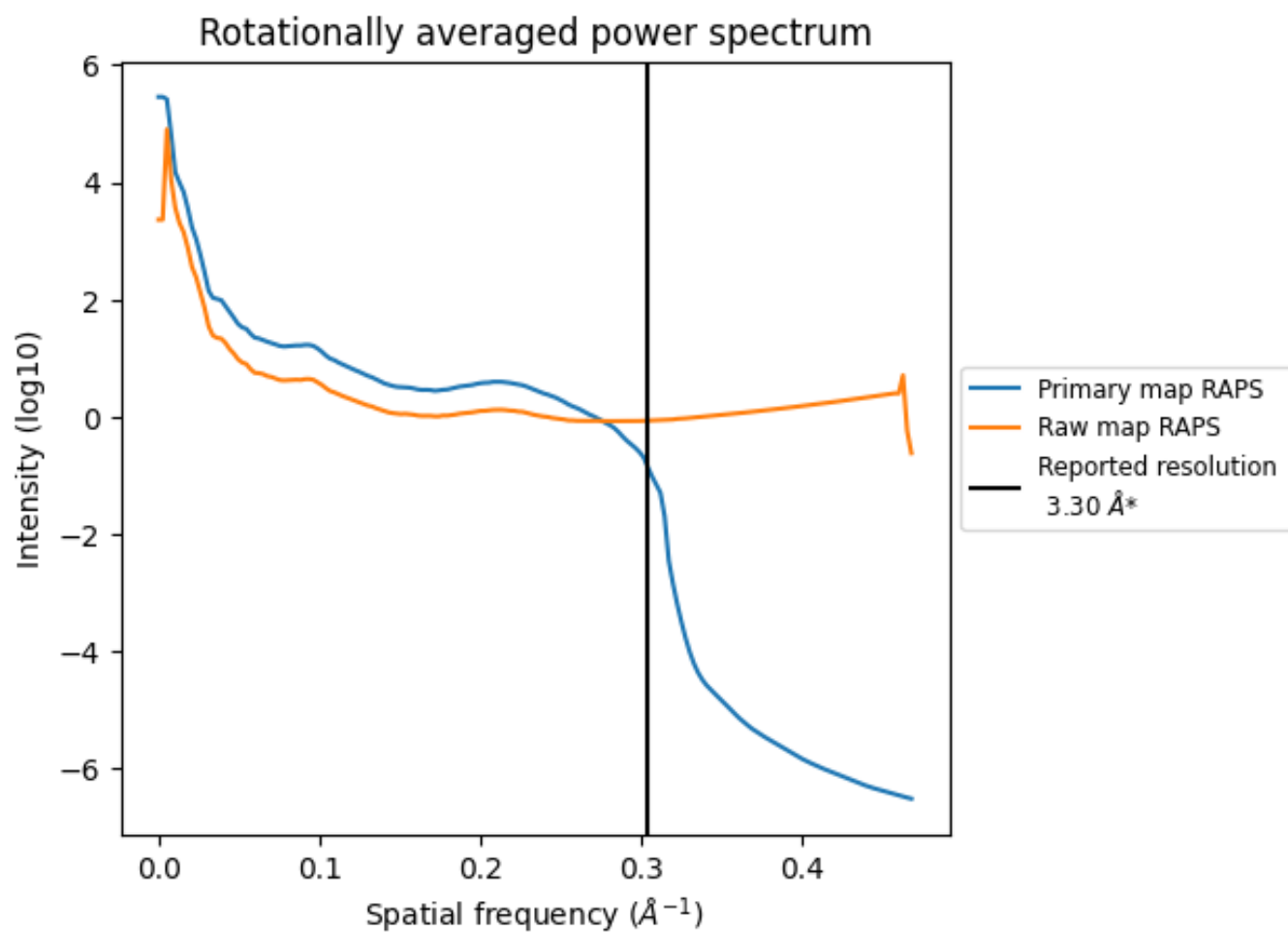
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 304 nm<sup>3</sup>; this corresponds to an approximate mass of 275 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

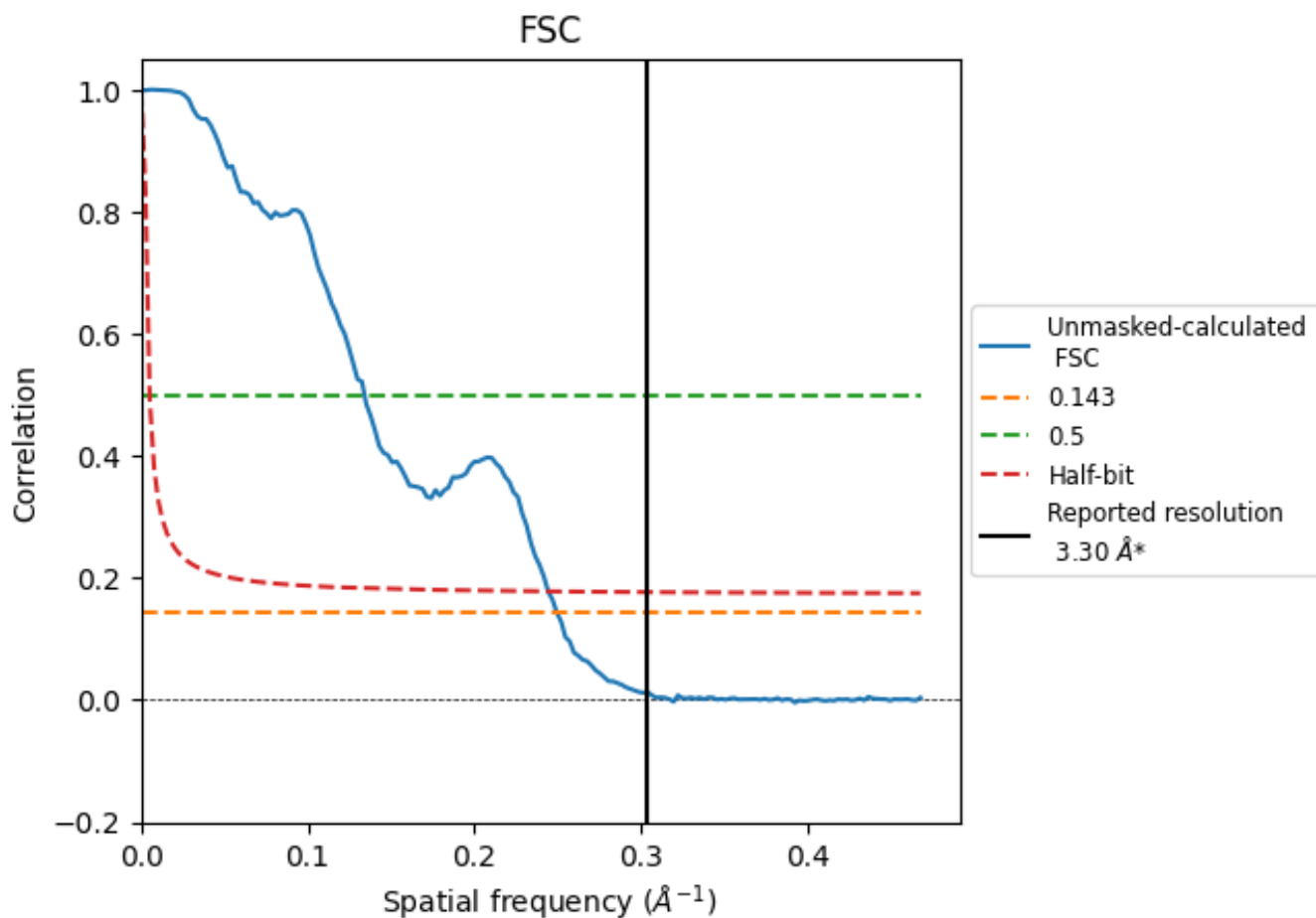


\*Reported resolution corresponds to spatial frequency of 0.303 Å<sup>-1</sup>

## 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](#)

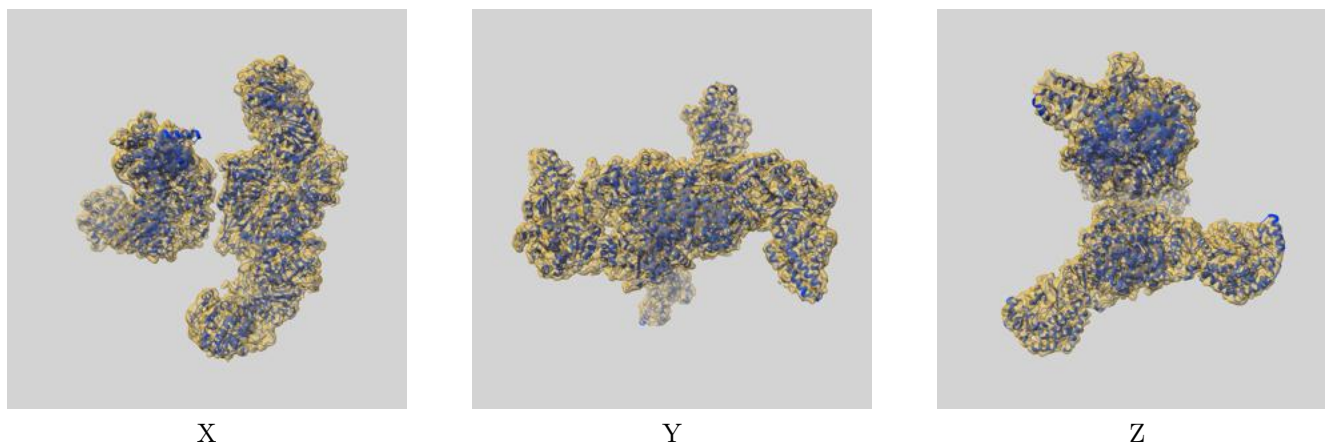
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.01	7.46	4.10

\*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 3.3 by more than 10 %

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

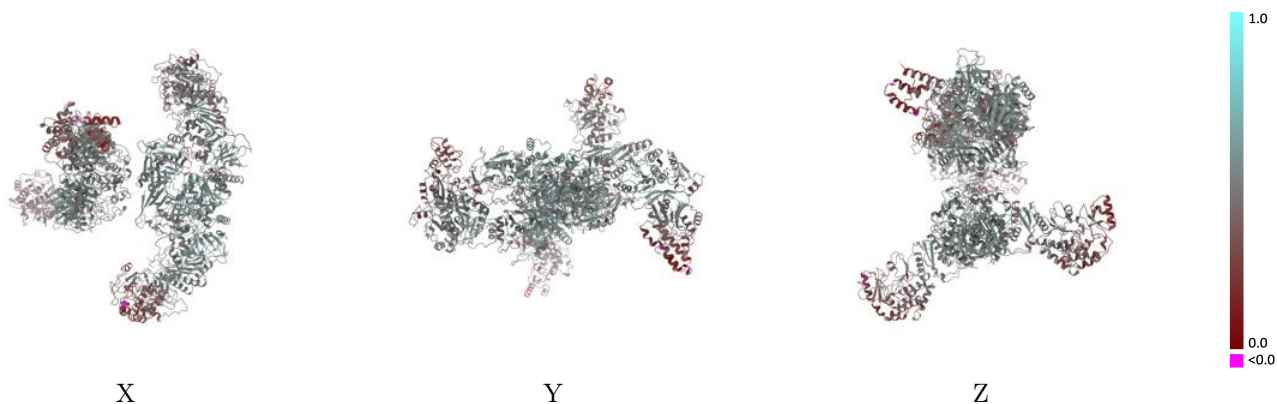
This section contains information regarding the fit between EMDB map EMD-43355 and PDB model 8VMC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

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



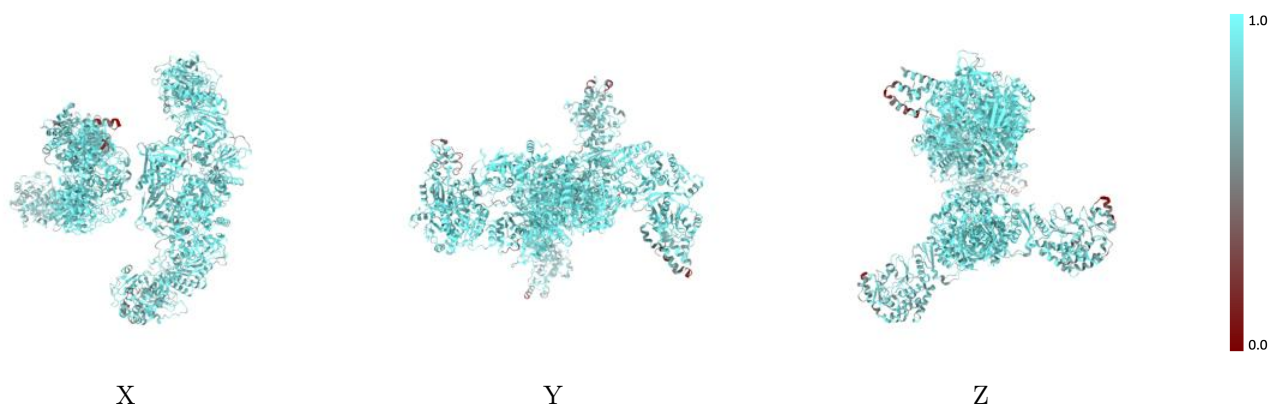
The images above show the 3D surface view of the map at the recommended contour level 0.173 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



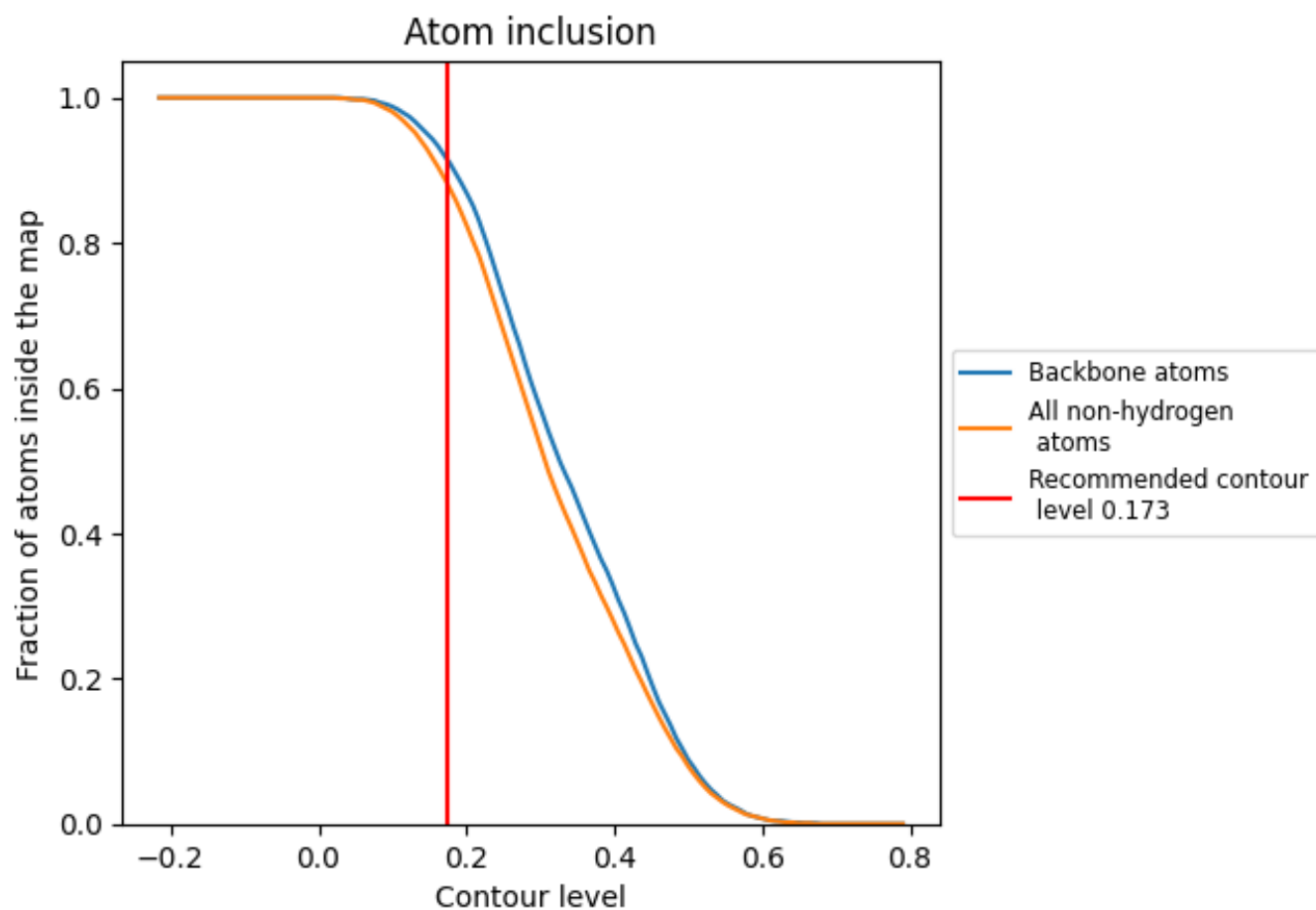
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.173).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 92% of all backbone atoms, 88% 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 (0.173) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8840	 0.4640
A	 0.8830	 0.4640
B	 0.8860	 0.4640

