



## wwPDB EM Validation Summary Report ⓘ

Feb 22, 2025 – 02:31 PM EST

PDB ID : 8VM5  
EMDB ID : EMD-43352  
Title : Composite structure of human FASN with NADPH in State 5  
Authors : Schultz, K.; Marmorstein, R.  
Deposited on : 2024-01-12  
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.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

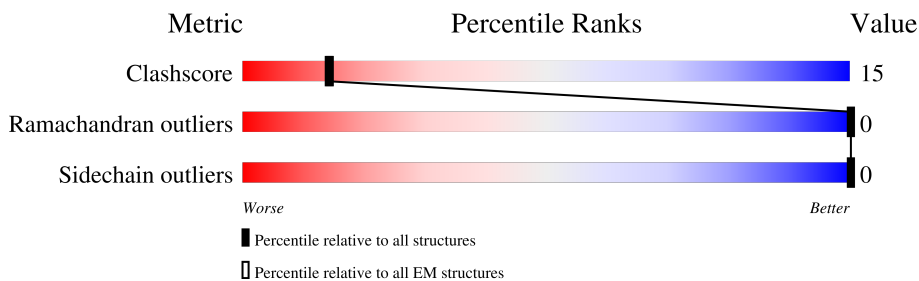
# 1 Overall quality at a glance

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	
1	B	2553	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 50709 atoms, of which 18827 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Fatty acid synthase.

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

There are 88 discrepancies between the modelled and reference sequences:

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

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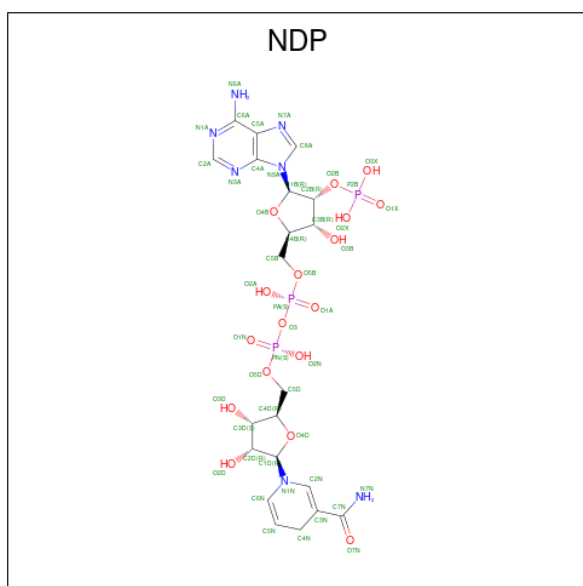
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP P49327
A	-4	MET	-	expression tag	UNP P49327
A	-3	GLY	-	expression tag	UNP P49327
A	-2	SER	-	expression tag	UNP P49327
A	-1	GLY	-	expression tag	UNP P49327
A	0	ILE	-	expression tag	UNP P49327
A	1	PRO	-	expression tag	UNP P49327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

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

- Molecule 2 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<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).

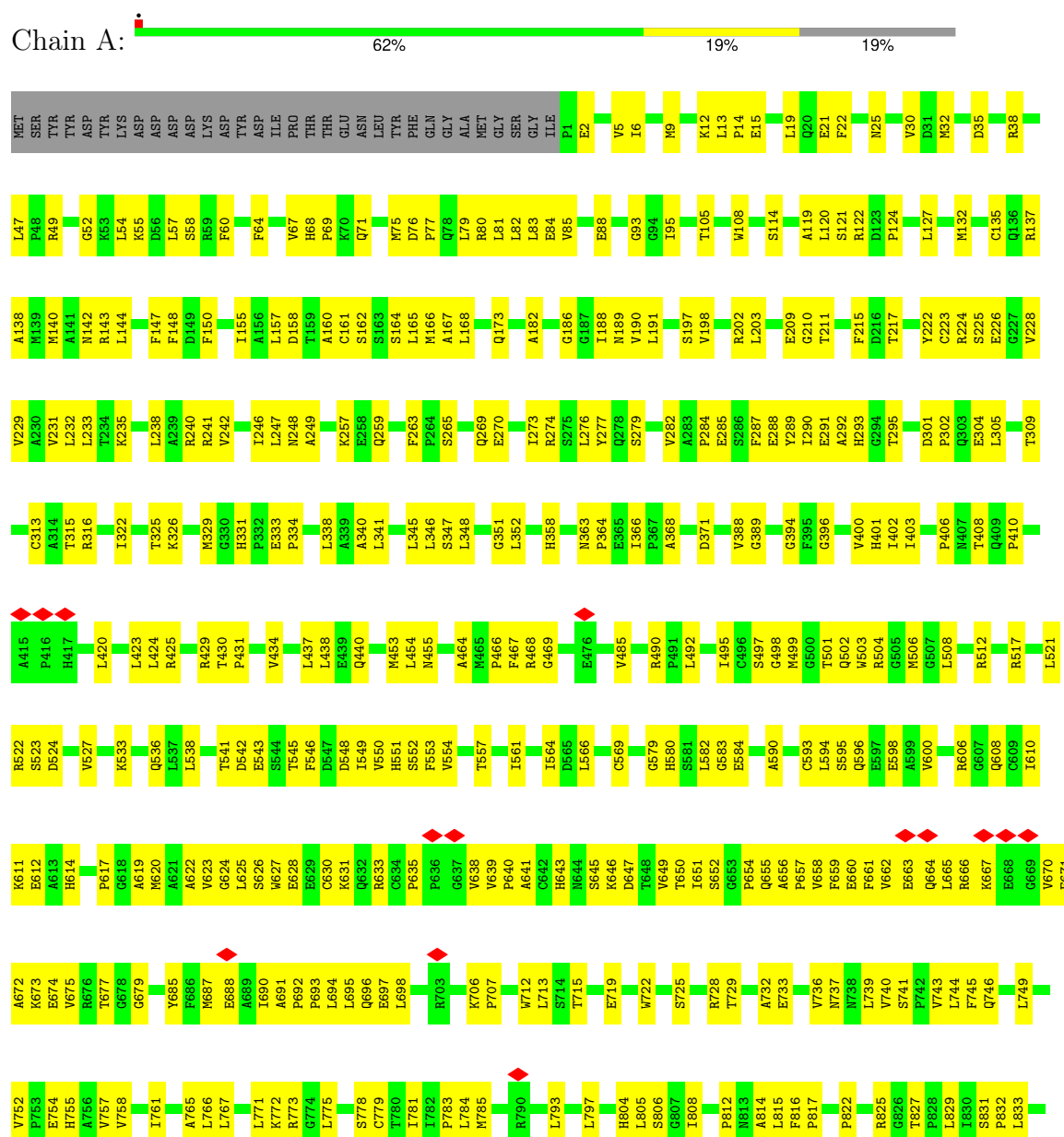


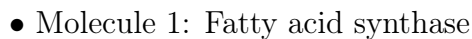
Mol	Chain	Residues	Atoms						AltConf
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	A	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	
2	B	1	Total	C	H	N	O	P	0
			74	21	26	7	17	3	

### 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



[illegible]



E2113	L1888	R1515	Y1270	C1141	L899	L767	L694	W627	V554	V472	A368	L276	V198
LYS	I1889	H1516	T1271	V1145	V912	Q768	L695	E628	S555	L473	L369	Y277	Q199
ALA	Q1902	F1517	A1272	V1145	V913	A769	Q696	E629	S555	E476	Q374	A283	F200
ALA	Q1906	E1521	T1273	T1150	V935	V770	L697	C630	T557	R477	Q375	P284	R202
ALA	D1274	E1521	D1274	THR	V935	K772	K699	Q832	A558		V376	E285	
ARG	R1907	T1535	R1275	VAL	E945	R773	K700	R633	I559	Q483	V377		M205
ASP	R1907	E1286	THR	THR	E945	G774	V701	R633	Q560	Q484		E288	L206
ASP	V1909	I1544	GLN	GLN	V958	L775	I702	P635	I561	V485		Y289	P208
ASP	Q1910		GLY			K776	R703	V638	I564			E291	E209
SER	K1911	R1582	LEU	LEU	T976	T780	P705	V639	D565	R490	P382	A292	G210
GLN	L1912	V1292	LYS	LYS	P977	I781	K706	P640	L566	P491	V383	H293	T211
ARG	Q1298	Q1293	MET	MET	N977	I782	P707	A641	L567	L492		G294	C212
ASP		Q1294	VAL	VAL	N978	P783	R708	C642	L567	F494	N391	T295	
LEU			VAL	VAL	E981				M570	I495	S392		F215
VAL	R1931	Y1568	PRO	PRO	P982	K786	S714	S645		C496	F393	D301	
GLY	W1932	L1571	GLY	GLY		K787	T715	K646	G576	S497		P302	G221
ALA		V1319	LEU	LEU	Y991	D788	S716	D647	I577	Q498	N399	Q303	C223
VAL	L1955	I1588	ASP	ASP		H789	I717	T648	V578	M499	V400	E304	C223
ALA		L1342	GLY	GLY	Q1006	G579	P718		G579		H401	L305	
HIS	L1980	T1593	ALA	ALA	G1007	L793	E719	I651	H580	G500	I402	R316	E226
ILE		S1594	ALA	ALA		G801	A720		S581	T501	I403		E226
ILE	S1997	Q1595	ILE	ILE	E1014				L582	Q502	L404		V228
GLY		Q1366	PRO	PRO		G807	L726		G583	V503	L404		
GLY		Q1369	ASP	ASP	R1019	H804	S806	P654	E584	R504	P406		
ILE	N2001	L1598	ASP	ASP	L1020	L805	G807	P657	G506	B504		L320	
ASP	S2020	L1616	GLY	GLY	L1021	S806	L726	V658	G507	G506	H417	I322	
LEU	S2021					G807	L726	G589	G507				T234
ALA		L1622	ALA	ALA	F1029	P812	A727	E660	L594		L420	T325	K235
VAL	Y2034	S1647	VAL	VAL	M1030	L815	R728	F661	L594	H511	R421	K326	K236
ASN		A1376	ASN	ASN	D1031	L815	T729	V662	Q596	L510	P421	S327	S237
LEU	E2042	V1650	LEU	LEU	T1032		A732	Q664	E597	R512	L424	M329	R240
ASP					Q1035	I830		L665	E597	R515	H331	R241	V242
SER	Q2059	V1680	SER	SER		S831	V736	R666			R429	P332	
SER		K1392	SER	SER	L1069	N737	N737	K667	L601	S523	R430	E333	T245
LEU	A2062	Q1714	LEU	LEU	A1199	L738	L739	E668	A602	D524	P431	P334	L246
ASP	L2063	ALA	ALA	ALA	Q1070	L739	L739	E668				A335	L247
ASP		V1417	ASP	ASP	D1071	V740	V740	G669	R606	V527	L437	S336	N248
LEU	V2066	S1775	LEU	LEU	K1072	S741	S741	V670	G607		L438	G337	A249
GLY		L1432	LEU	LEU	A1073	P742	P742	F671	Q608	L532	L438	L338	G250
LEU	ILE	I1446	LEU	LEU	Q1074	V743	V743	A672	G609	L532	Q440	L338	T251
ASP	ASP	I1446	ASP	ASP	V1078	L744	L744	K673	E610	K533	Q440	A340	N252
LEU	VAL	S1451	LEU	LEU	V1079	GLY	GLY	E874	K611	V534			T253
SER	GLU	C1452	SER	SER	V1080	SER	SER	E874	E612		R443	K343	D254
THR	THR	V1453	THR	THR	V1080	PRO	PRO		E612			V344	G255
MET	MET	V1457	MET	MET	T1087	SER	SER					S347	F256
SER	SER	V1457	SER	SER	T1088	A859	A859					L348	F256
VAL	VAL	G1471	VAL	VAL	A1089	Y862	P753	H683	L615	L615	L454	L348	E258
VAL	VAL	C1471	VAL	VAL	A1089	Y862	P753	H683	L615	L615	L454	L348	Q259
ARG	ARG	L1474	ARG	ARG	Q1110	T879	H755	Y685	G618	D542	V460	G351	G260
GLN	THR	L1474	GLN	GLN	V1111	L880	A756	Y685	G618	E543	P461	A354	V261
THR	THR	V1853	THR	THR	T1120	L880	V757	M687	M620	T545	A354	A354	T262
LEU	LEU	E1485	LEU	LEU	T1120	T889	V758	E688	A821	F546	A464	P355	F263
GLU	GLU	V1486	GLU	GLU	E1125	T889	L759	A689	A622	D547	N356	N356	F263
ARG	S2081	A1868	ARG	ARG	E1125	I894	E760	I690	G624	D548	F467	E270	E270
GLY		T1879	GLY	GLY	E1130	I894	E760	I690	G624	D548	F467	E270	E270
LEU	P2085		LEU	LEU	E1130	T898	A765	A691	L625	I549	R468	E365	R274
ASN	L2097	A1883	ASN	ASN	E1130	T898	A765	A691	L625	I549	R468	E365	R274
							L766	P693	S626	H551	A471	P367	S275

VAL	ARG	ASP	ARG	ALA	CYS
SER	ARG	ILE	ALA	ILE	ILE
VAL	LEU	GLN	LYS	ARG	ARG
HIS	GLU	LEU	LEU	GLN	THR
VAL	THR	VAL	THR	VAL	VAL
ILE	SER	SER	PRO	GLN	GLY
GLU	PHE	GLY	PRO	PRO	GLY
GLY	ALA	CYS	GLU	GLY	VAL
ASP	ALA	GLY	GLU	GLY	VAL
HIS	ARG	ALA	PRO	ARG	GLN
ARG	SER	SER	GLU	GLU	THR
THR	PHE	ALA	ALA	VAL	LEU
LEU	TYR	TYR	GLU	GLU	LEU
LEU	TYR	THR	THR	THR	ARG
GLU	LYS	LEU	GLU	GLY	LYS
GLY	SER	ARG	ILE	ILE	GLN
LEU	ALA	ALA	ILE	ARG	GLN
LEU	GLY	ALA	CYS	TYR	LEU
GLU	ALA	GLY	PHE	GLY	SER
SER	GLU	GLN	VAL	ALA	GLY
ILE	THR	THR	VAL	CYS	SER
ILE	THR	PRO	GLN	VAL	LYS
ILE	SER	PHE	GLN	ALA	ALA
ILE	ILE	THR	ALA	THR	ASP
ILE	THR	ASP	THR	GLU	GLU
HIS	LYS	MET	MET	GLU	ALA
SER	LYS	CYS	SER	GLY	ALA
SER	TYR	SER	GLU	THR	GLY
LEU	HIS	HIS	GLN	LEU	LEU
LEU	GLY	ASN	ASN	LEU	ALA
ALA	ASN	ARG	VAL	ARG	CYS
GLU	VAL	VAL	LEU	VAL	PRO
PRO	MET	LEU	GLU	GLN	THR
ARG	VAL	LEU	ALA	GLN	PRO
VAL	VAL	LEU	ALA	SER	LYS
SER	SER	ARG	LEU	PRO	GLU
VAL	VAL	ALA	LEU	ALA	ASP
ARG	ARG	LYS	PRO	PRO	TYR
GLU	GLY	THR	LEU	THR	GLY
LEU	GLY	GLY	LYS	HIS	LEU
GLU	LEU	ALA	GLY	ASN	ALA
HIS	GLY	TYR	LEU	SER	GLN
HIS	GLY	GLY	GLU	LEU	THR
HIS	GLU	THR	GLU	PHE	ARG
HIS	HIS	GLY	ARG	LEU	GLN
HIS	HIS	VAL	VAL	PHE	ALA
HIS	HIS	LEU	ALA	ASP	ALA
HIS	HIS	GLY	ALA	GLY	PRO
HIS	HIS	ALA	ALA	LEU	LEU
HIS	ASP	VAL	VAL	SER	ARG
HIS	TYR	ASP	ASP	PRO	SER
HIS	ASN	THR	THR	PRO	LEU
HIS	LEU	LEU	TYR	ILE	LEU
HIS	ILE	VAL	VAL	HIS	ASN
HIS	SER	LEU	LEU	SER	VAL
HIS	GLN	GLN	LYS	ALA	PRO
HIS	VAL	THR	ALA	ALA	GLY
HIS	CYS	SER	THR	ALA	GLY
HIS	ASP	HIS	THR	ALA	PRO
HIS	GLY	GLN	GLN	THR	THR
HIS	GLY	GLY	SER	ILE	THR
HIS	LYS	LEU	LEU	ASP	LEU

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	157272	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	0.741	Depositor
Minimum map value	-0.185	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.161	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	0.28	0/16198	0.48	0/22023
1	B	0.28	0/16222	0.48	0/22055
All	All	0.28	0/32420	0.48	0/44078

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

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	468	0
1	B	15857	9380	15826	523	0
2	A	96	52	52	2	0
2	B	96	52	52	5	0
All	All	31882	18827	31739	970	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 970 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:292:ALA:HB2	1:B:322:ILE:HD11	1.36	1.08
1:A:164:SER:HB2	1:A:338:LEU:HD13	1.39	1.03
1:B:619:ALA:HB3	1:B:658:VAL:HG11	1.38	1.02
1:A:687:MET:HE2	1:A:739:LEU:HD11	1.38	1.02
1:A:725:SER:HA	1:A:728:ARG:HH12	1.24	1.02

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%)	1994 (97%)	66 (3%)	0	100	100
1	B	2063/2553 (81%)	2002 (97%)	61 (3%)	0	100	100
All	All	4123/5106 (81%)	3996 (97%)	127 (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%)	1708 (100%)	0	100	100
All	All	3413/4234 (81%)	3413 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
1	A	664	GLN
1	B	78	GLN
1	B	195	ASN
1	B	580	HIS
1	B	1345	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NDP	B	2602	-	47,52,52	0.67	0	61,80,80	0.80	2 (3%)
2	NDP	A	2601	-	47,52,52	0.65	0	61,80,80	0.85	3 (4%)
2	NDP	B	2601	-	47,52,52	0.66	0	61,80,80	0.93	2 (3%)
2	NDP	A	2602	-	47,52,52	0.65	0	61,80,80	0.81	3 (4%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NDP	B	2602	-	-	11/30/77/77	0/5/5/5
2	NDP	A	2601	-	-	14/30/77/77	0/5/5/5
2	NDP	B	2601	-	-	8/30/77/77	0/5/5/5
2	NDP	A	2602	-	-	11/30/77/77	0/5/5/5

There are no bond length outliers.

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2601	NDP	P2B-O2B-C2B	-5.30	109.26	123.43
2	B	2602	NDP	P2B-O2B-C2B	-3.55	113.94	123.43
2	A	2602	NDP	P2B-O2B-C2B	-3.35	114.49	123.43
2	A	2601	NDP	C4B-O4B-C1B	-2.60	107.54	109.92
2	B	2601	NDP	C5A-C6A-N6A	2.29	123.79	120.31

There are no chirality outliers.

5 of 44 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-O7N
2	A	2602	NDP	C5B-O5B-PA-O2A
2	A	2602	NDP	C5B-O5B-PA-O3

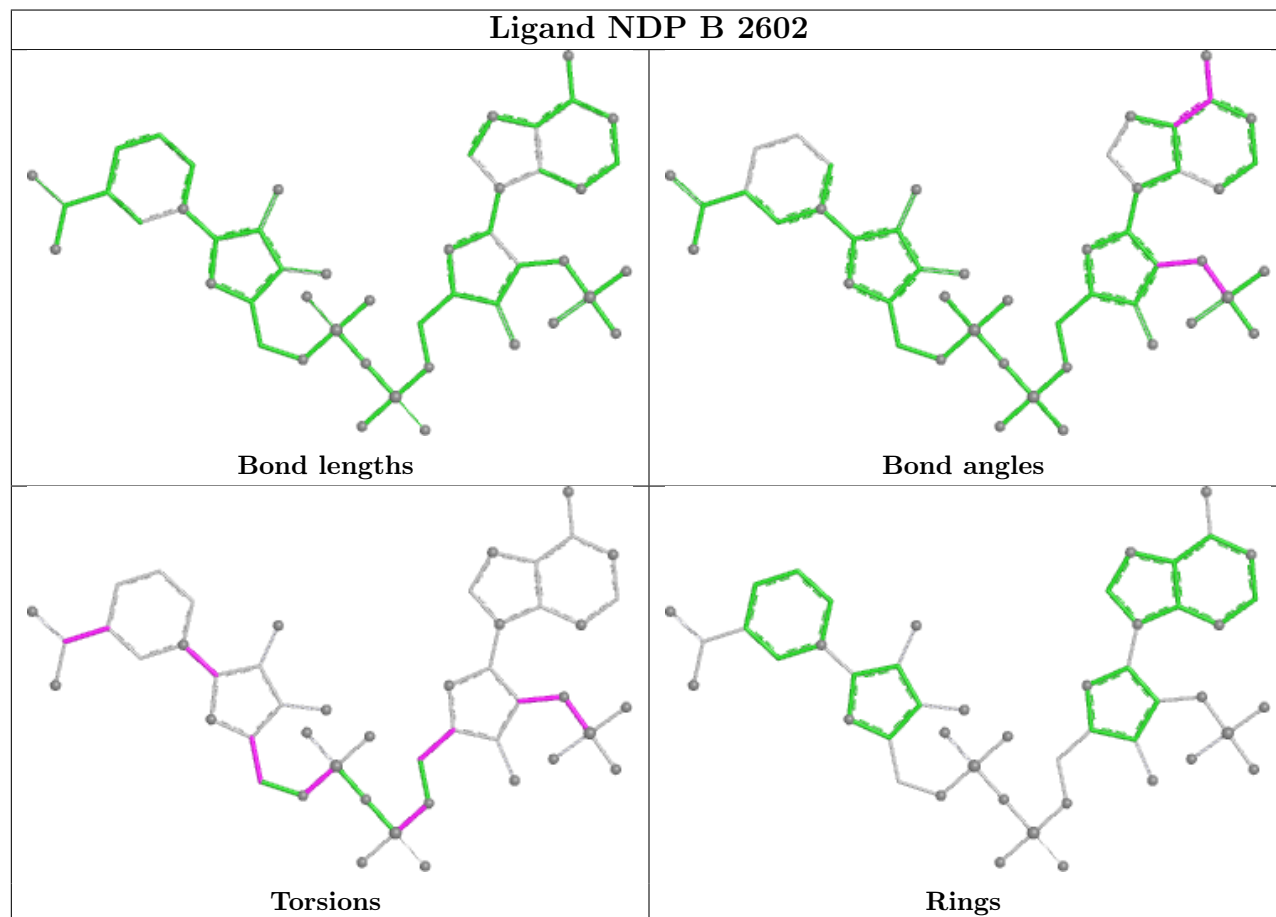
There are no ring outliers.

4 monomers are involved in 7 short contacts:

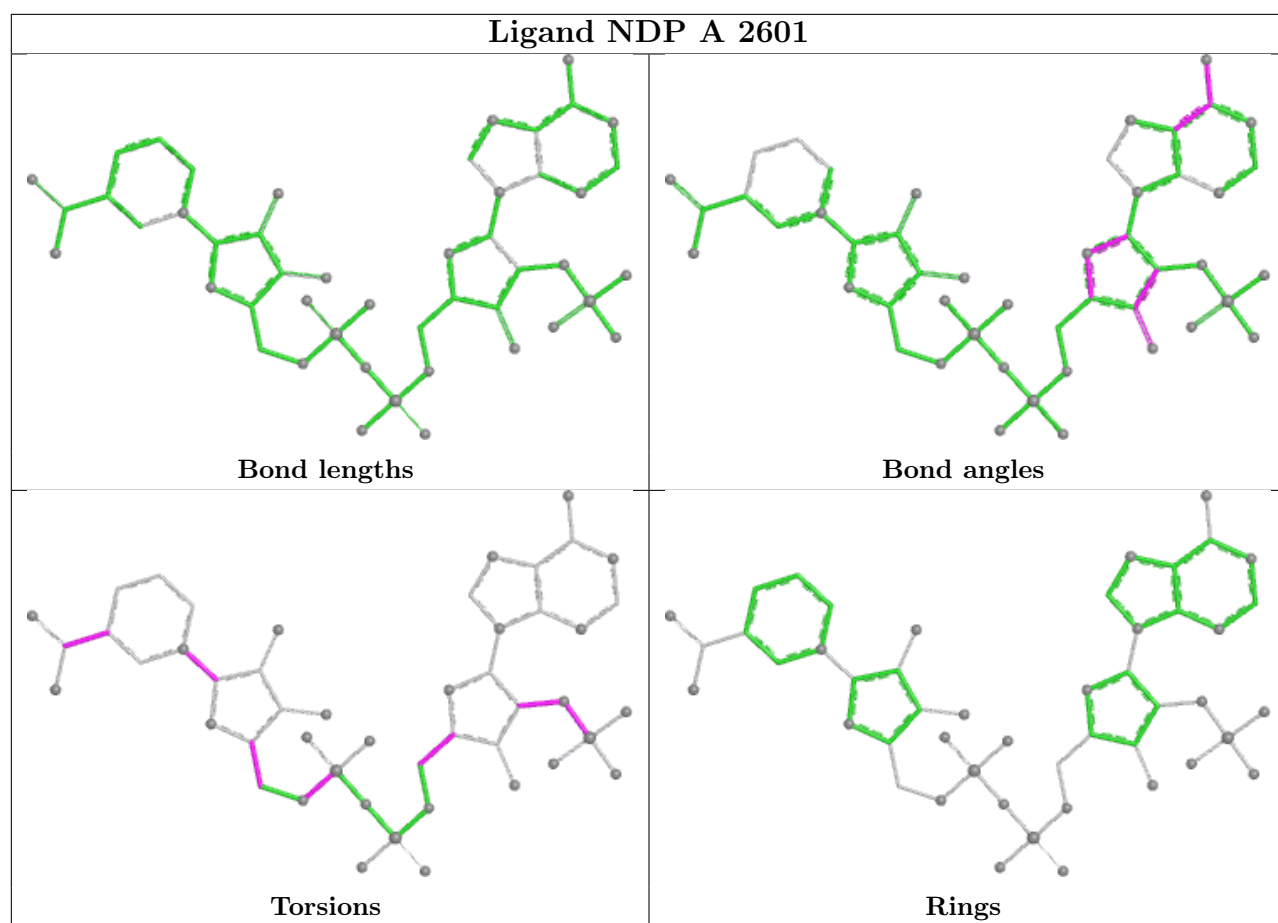
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2602	NDP	1	0
2	A	2601	NDP	1	0
2	B	2601	NDP	4	0
2	A	2602	NDP	1	0

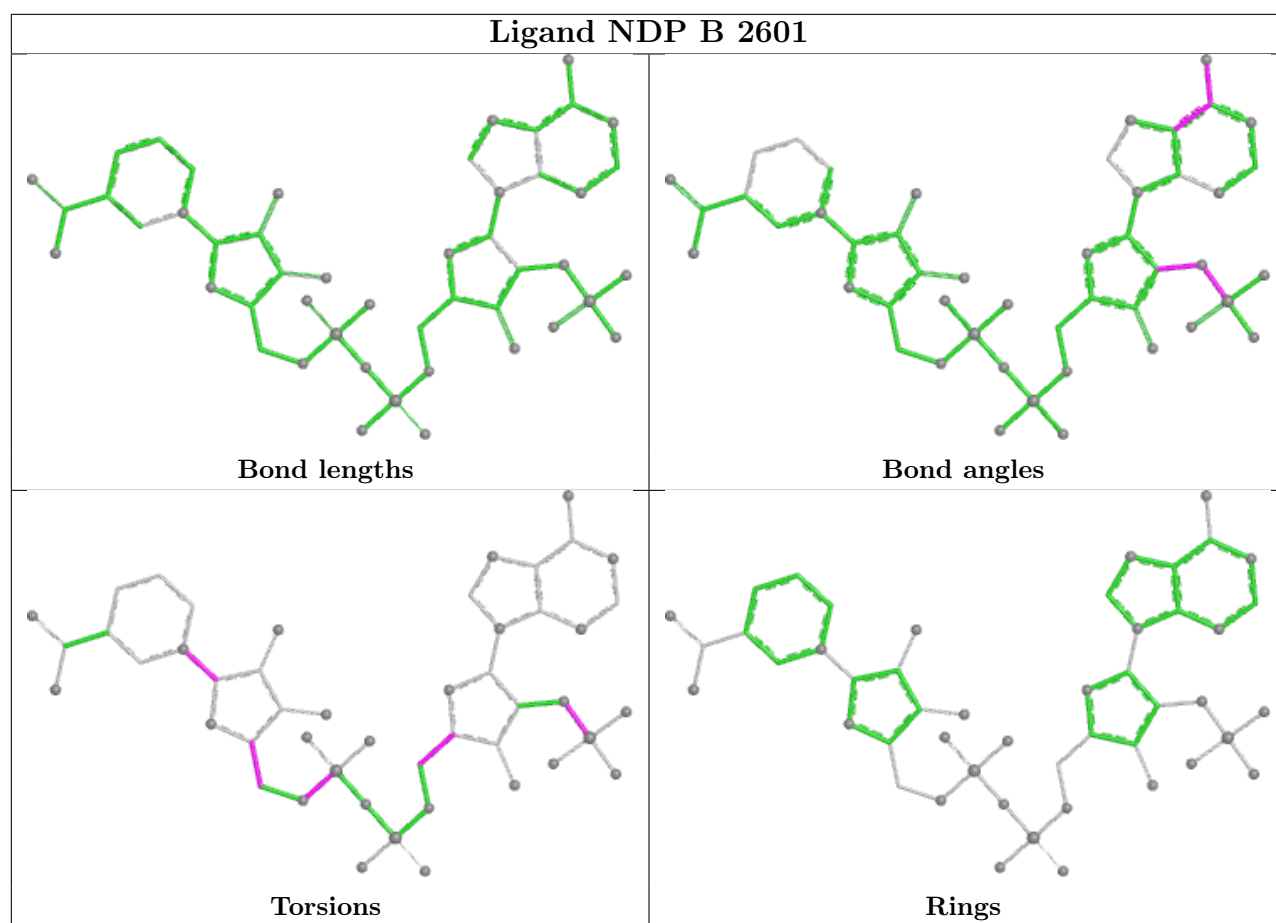
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

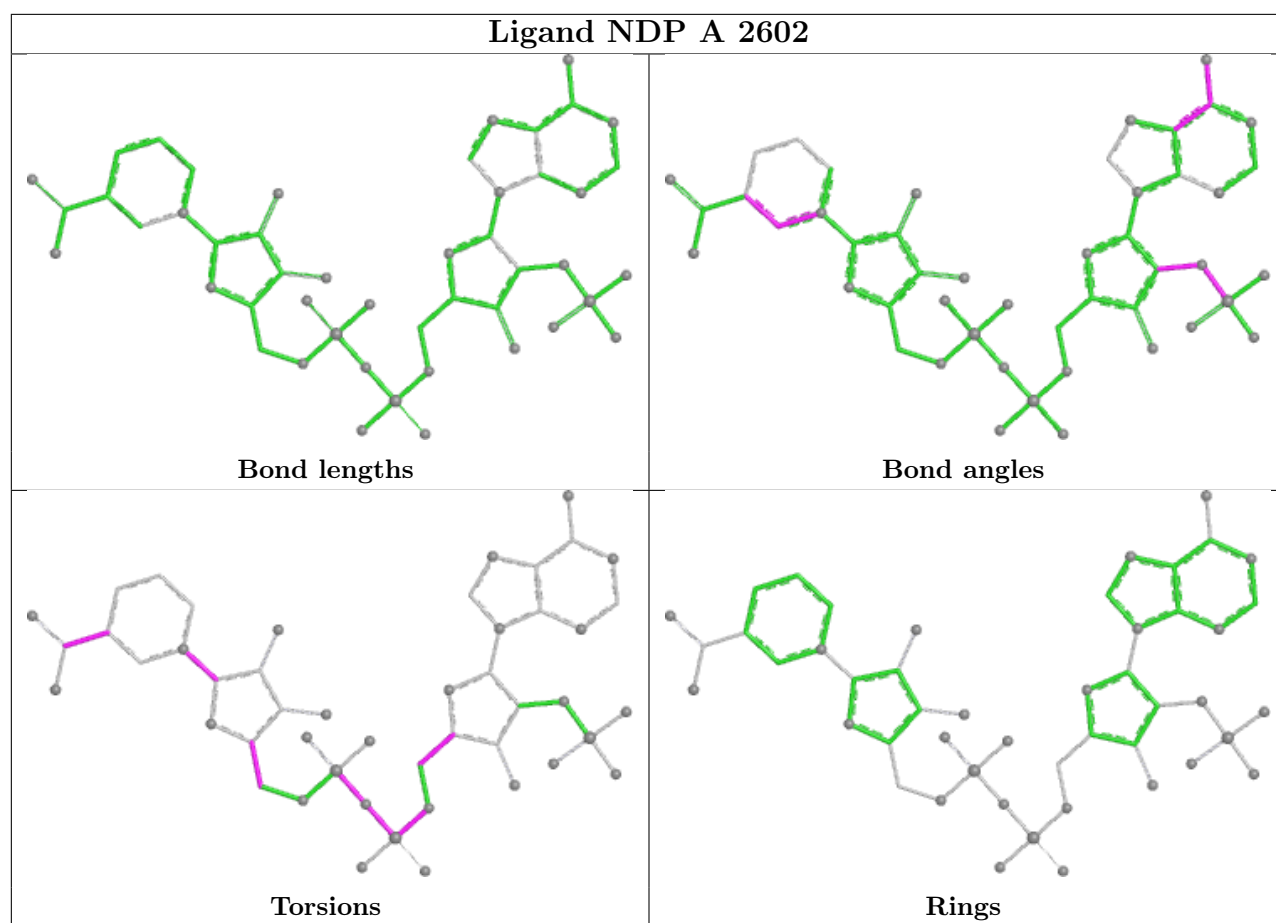
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. 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.

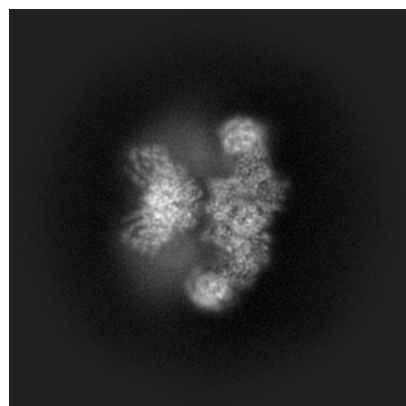
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43352. These allow visual inspection of the internal detail of the map and identification of artifacts.

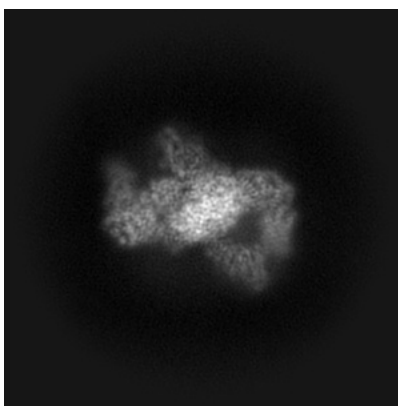
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

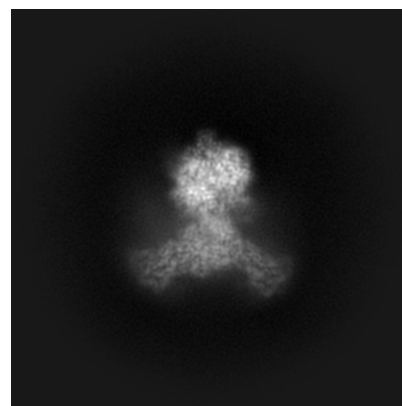
#### 6.1.1 Primary map



X

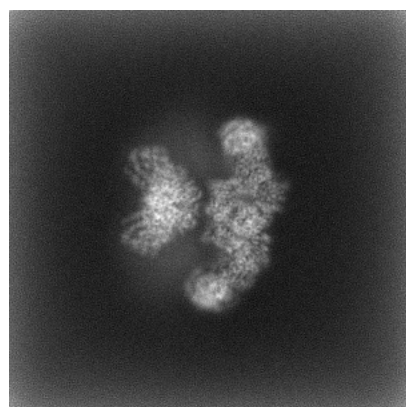


Y

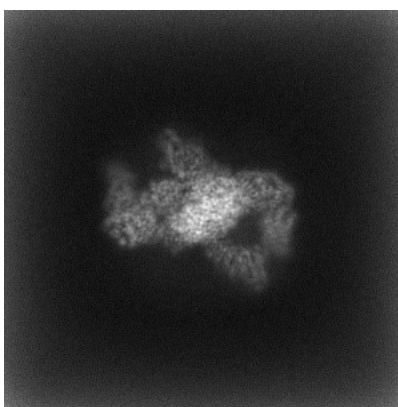


Z

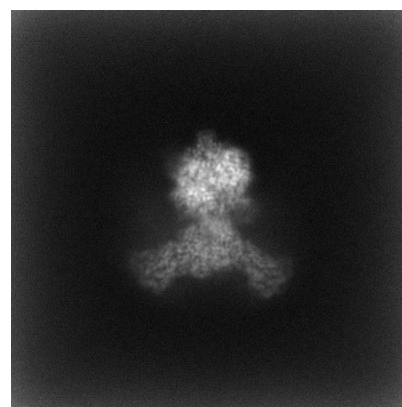
#### 6.1.2 Raw map



X



Y

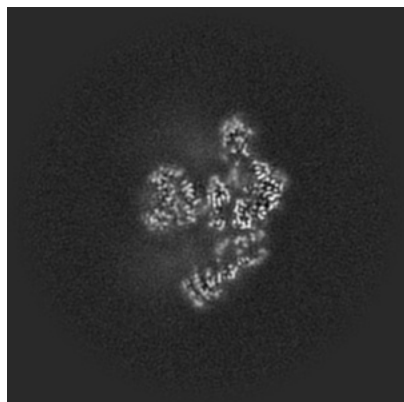


Z

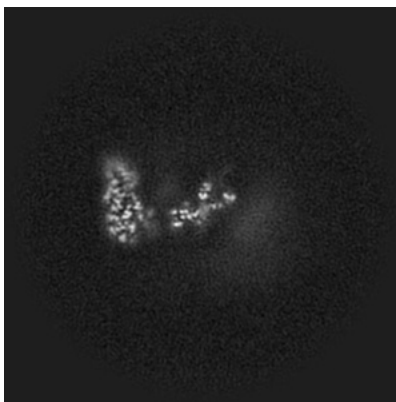
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

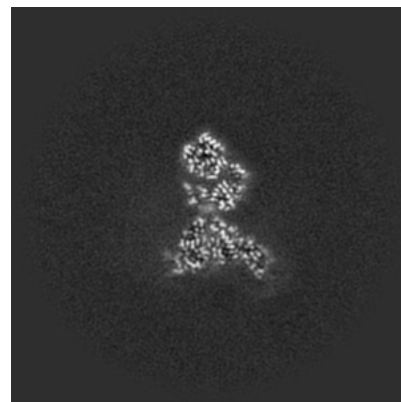
### 6.2.1 Primary map



X Index: 180

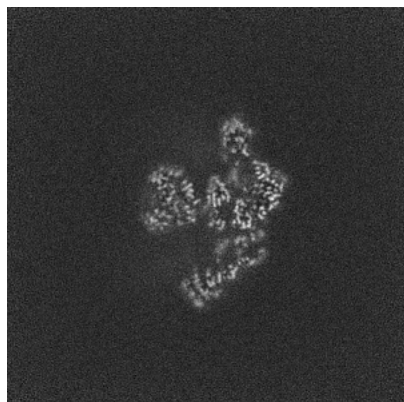


Y Index: 180



Z Index: 180

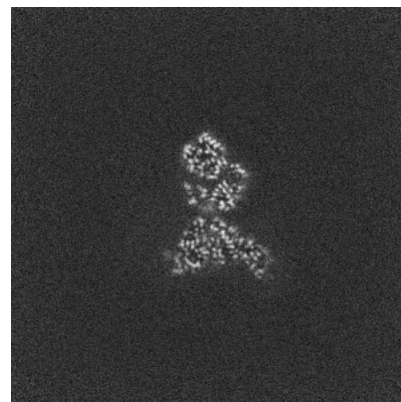
### 6.2.2 Raw map



X Index: 180



Y Index: 180

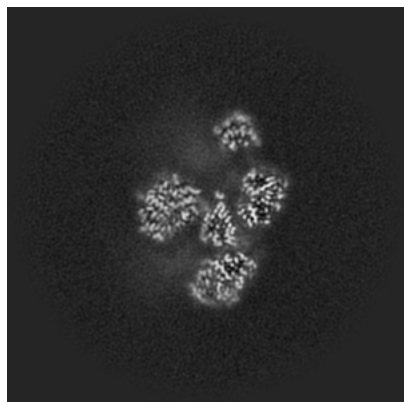


Z Index: 180

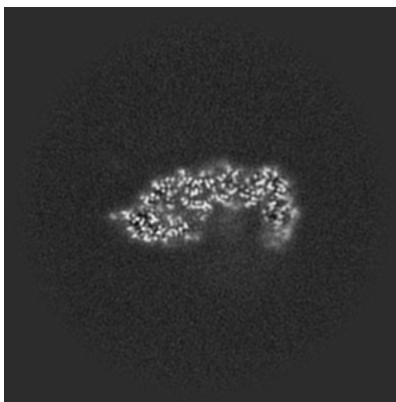
The images above show central slices of the map in three orthogonal directions.

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

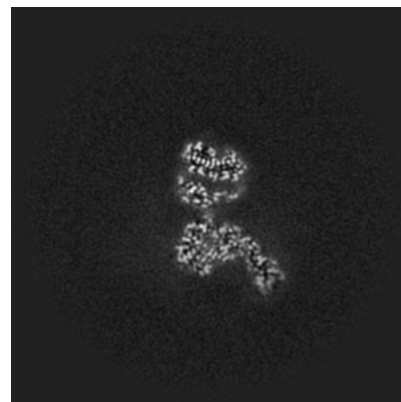
### 6.3.1 Primary map



X Index: 173

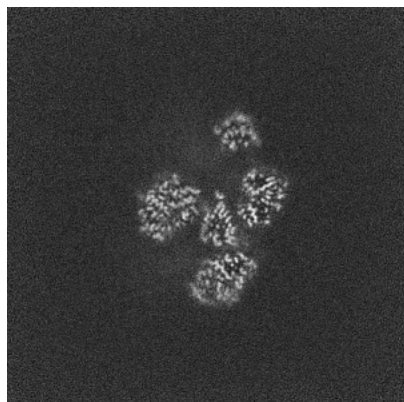


Y Index: 207

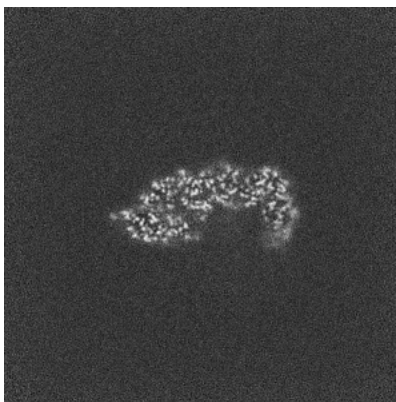


Z Index: 173

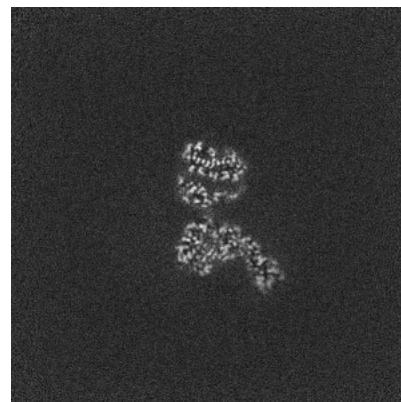
### 6.3.2 Raw map



X Index: 173



Y Index: 207



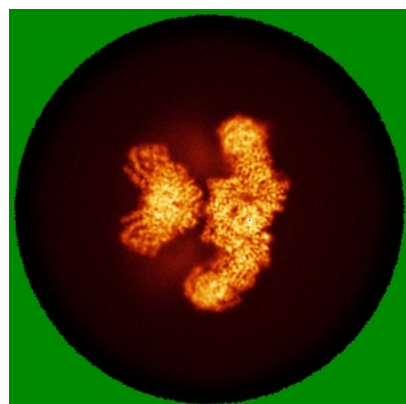
Z Index: 173

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

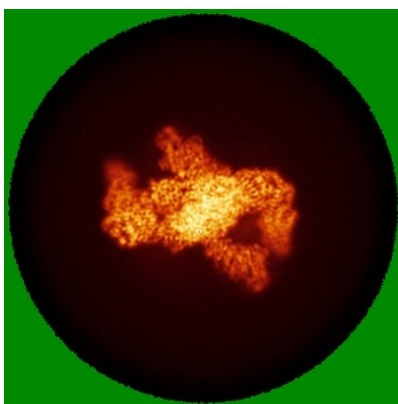


## 6.4 Orthogonal standard-deviation projections (False-color) [i](#)

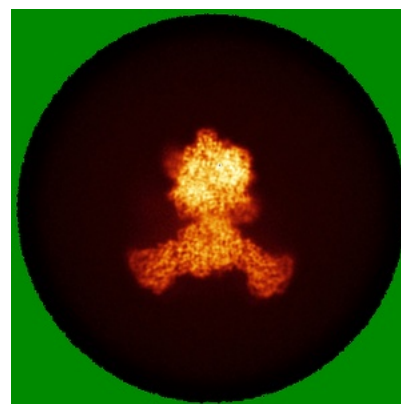
### 6.4.1 Primary map



X

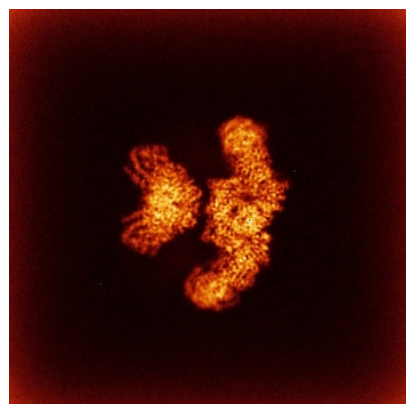


Y

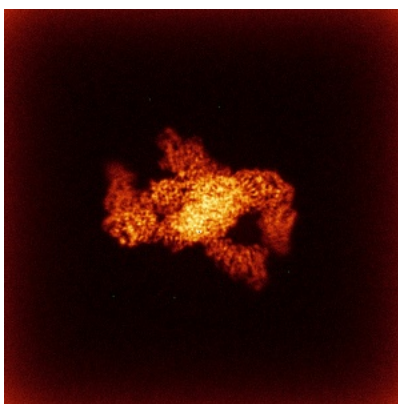


Z

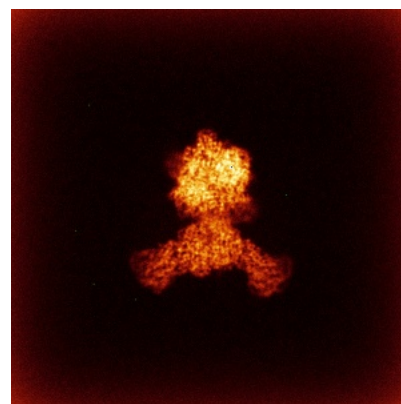
### 6.4.2 Raw map



X



Y



Z

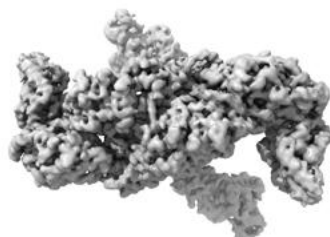
The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

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

### 6.5.1 Primary map



X



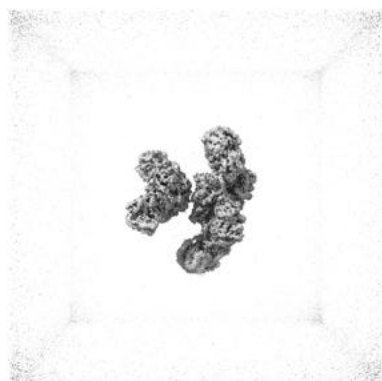
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.161. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

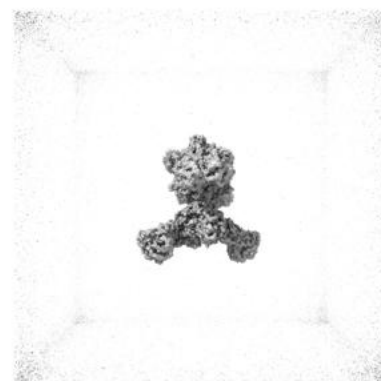
### 6.5.2 Raw map



X



Y



Z

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.



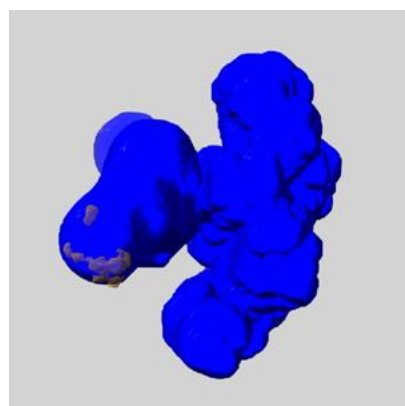
## 6.6 Mask visualisation [i](#)

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

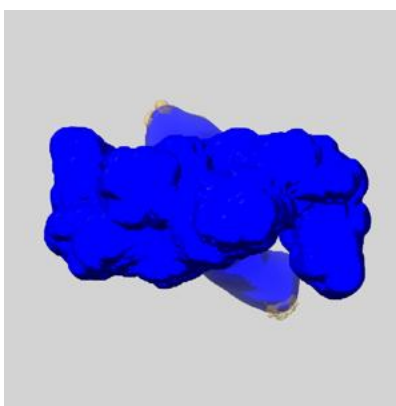
A mask typically either:

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

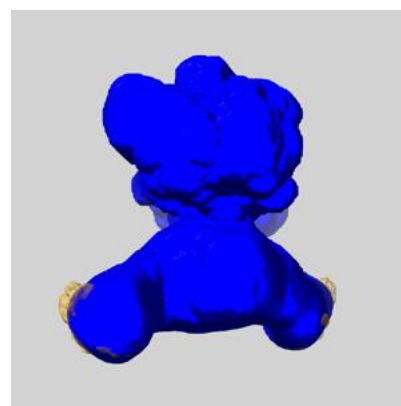
### 6.6.1 emd\_43352\_msk\_1.map [i](#)



X



Y

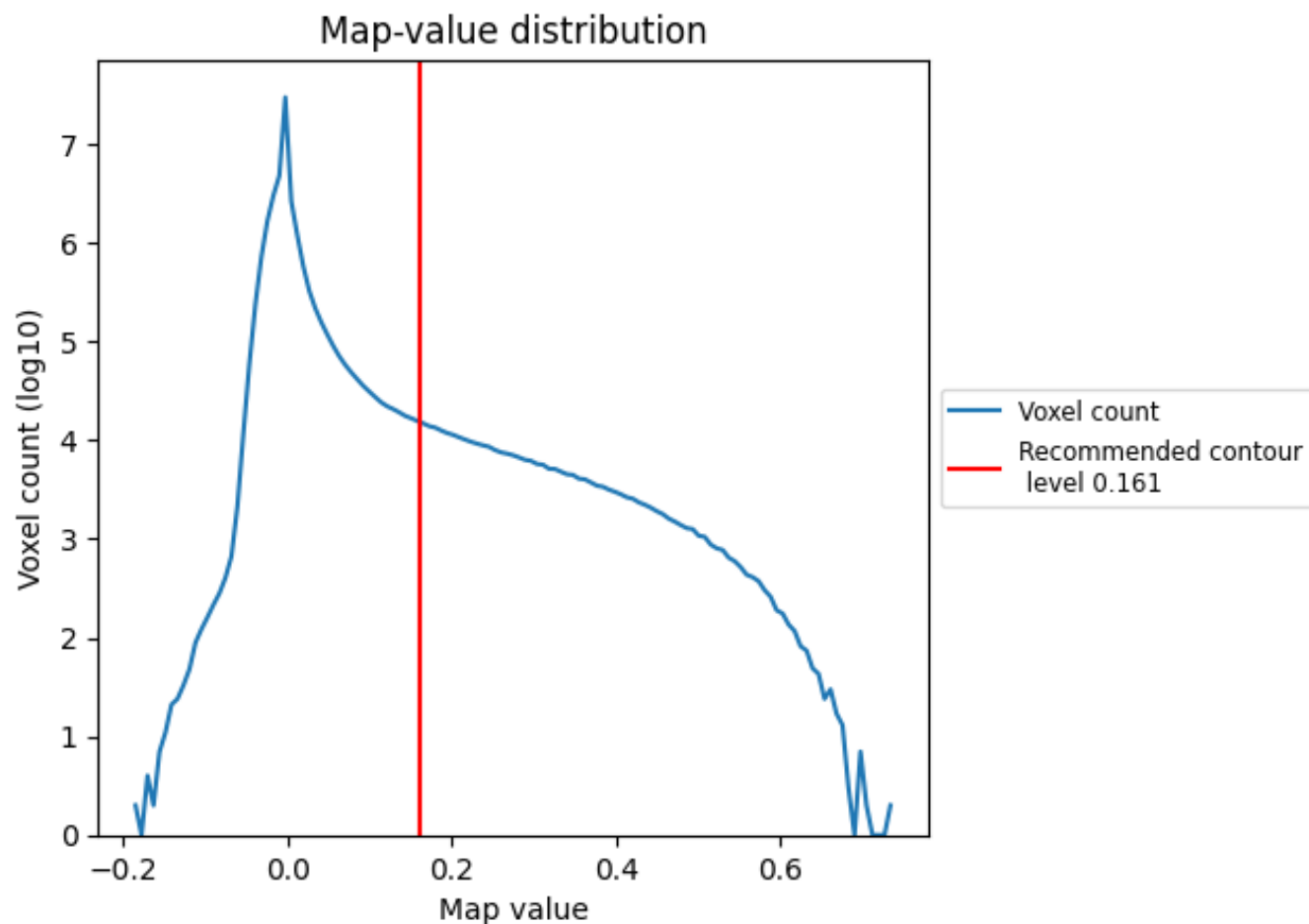


Z

## 7 Map analysis [i](#)

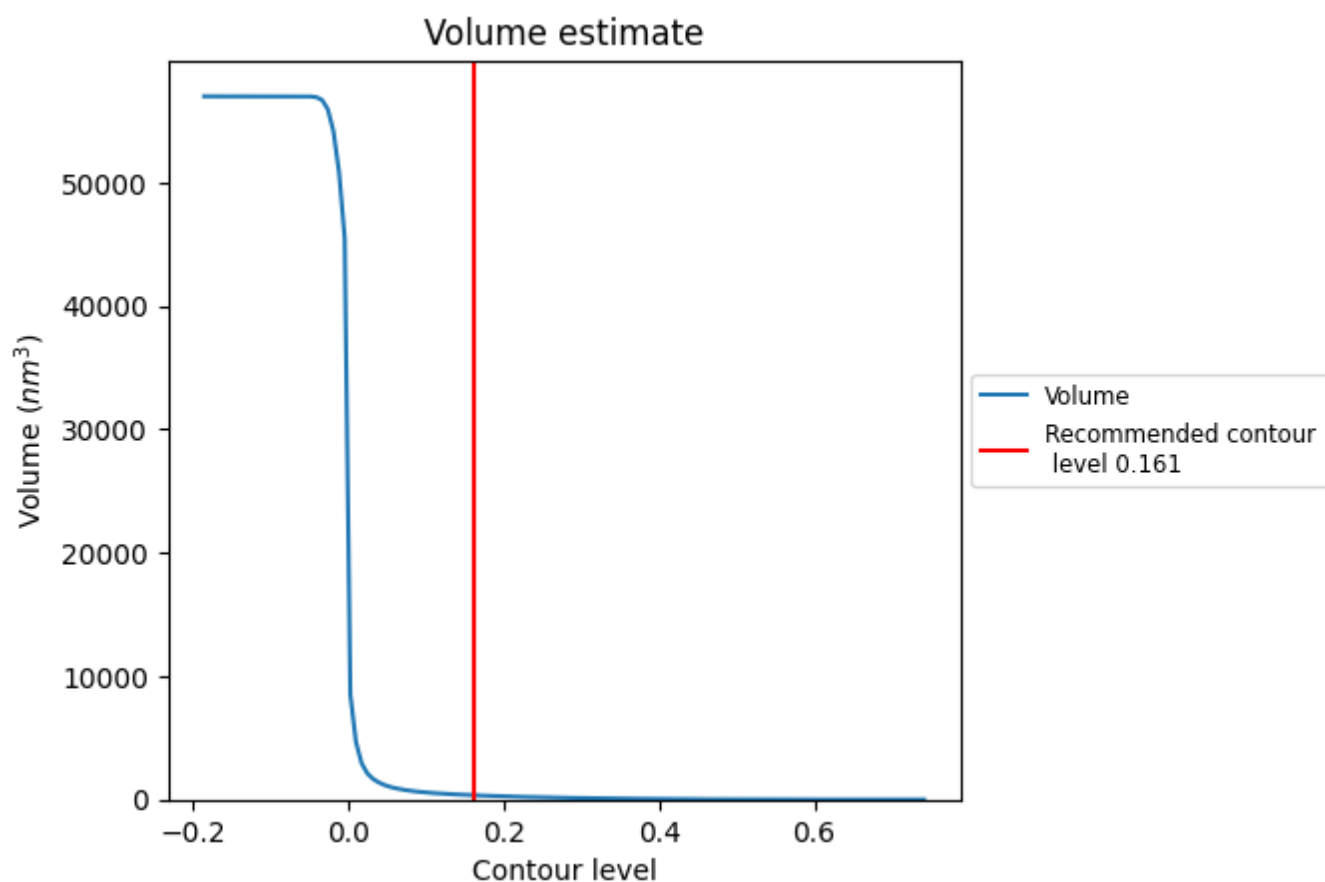
This section contains the results of statistical analysis of the map.

### 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.

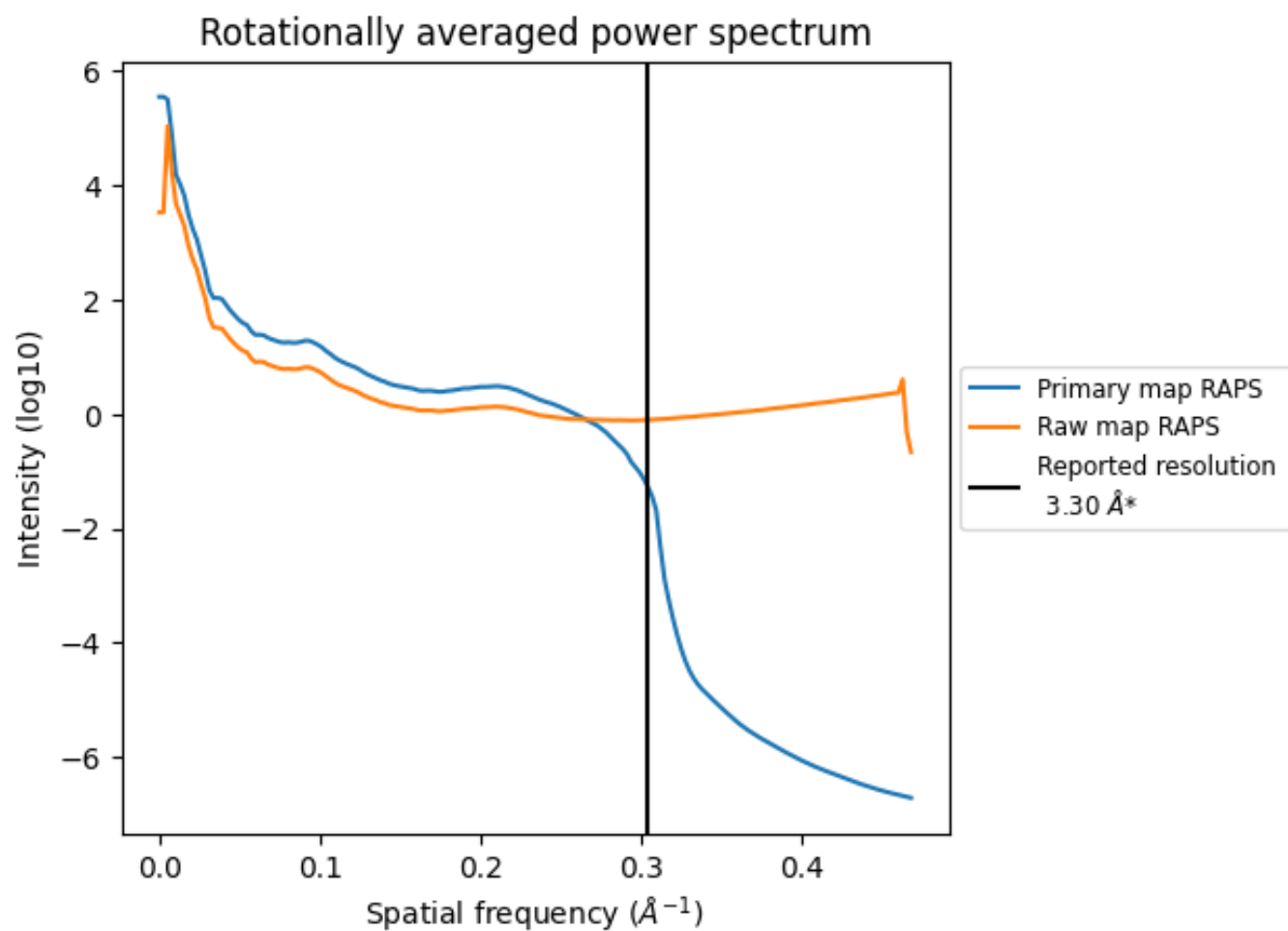
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 352 nm<sup>3</sup>; this corresponds to an approximate mass of 318 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 ⓘ

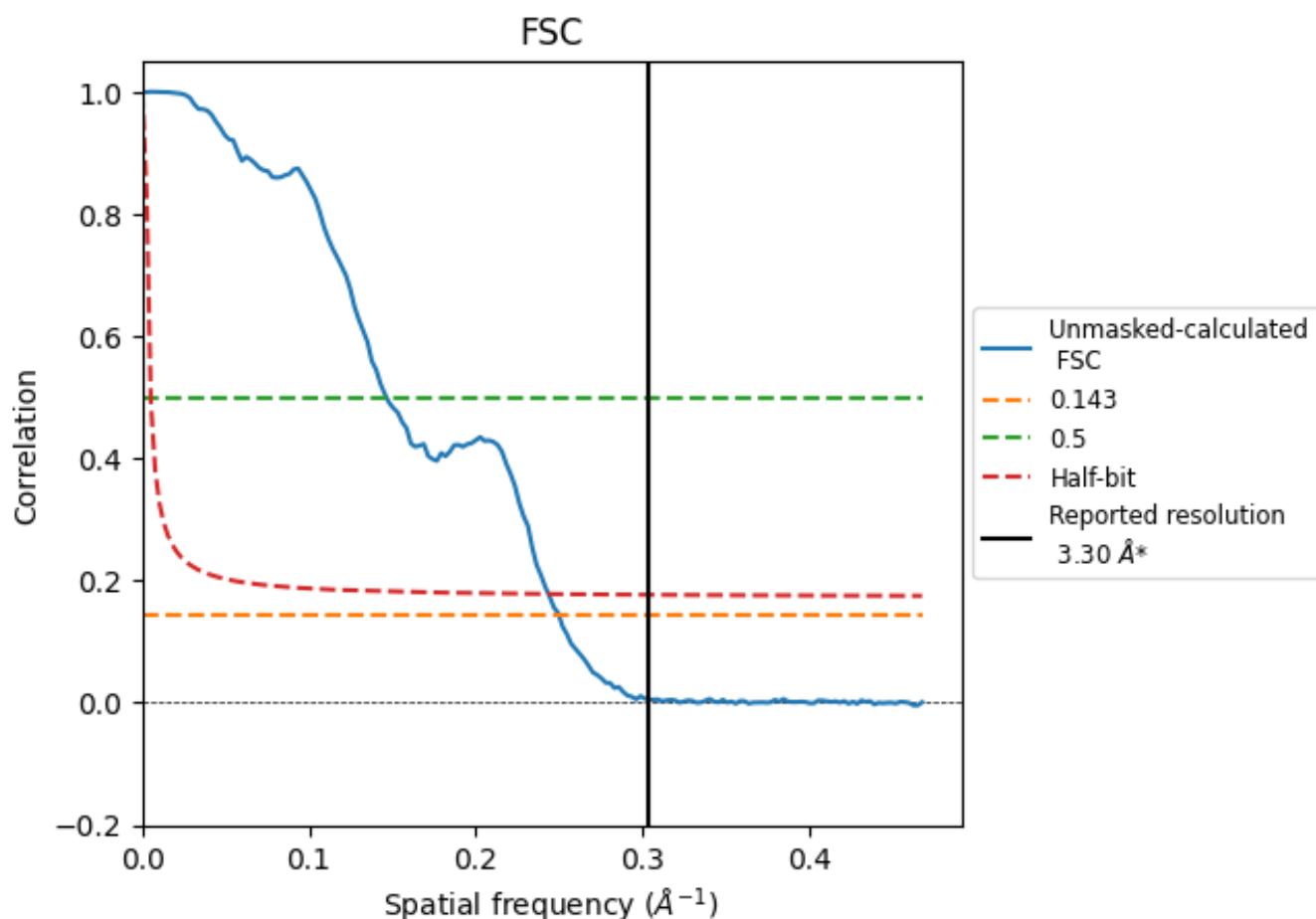


\*Reported resolution corresponds to spatial frequency of 0.303  $\text{\AA}^{-1}$

## 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](#)

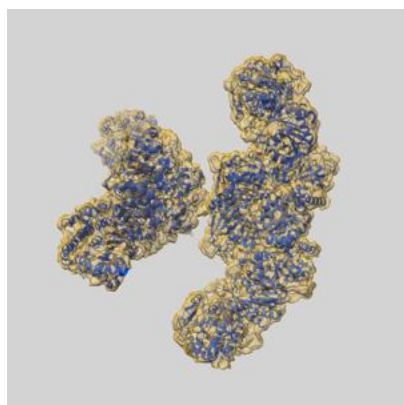
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.30	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.00	6.83	4.11

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.00 differs from the reported value 3.3 by more than 10 %

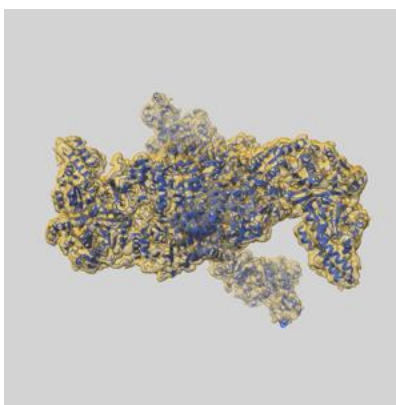
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43352 and PDB model 8VM5. Per-residue inclusion information can be found in section [3](#) on page [7](#).

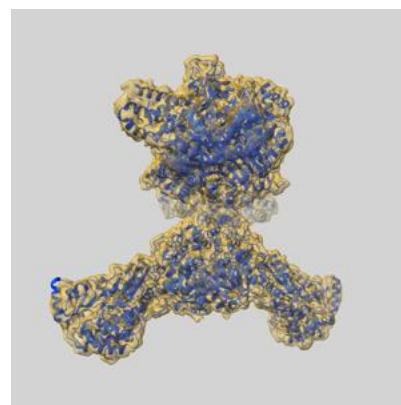
### 9.1 Map-model overlay [i](#)



X



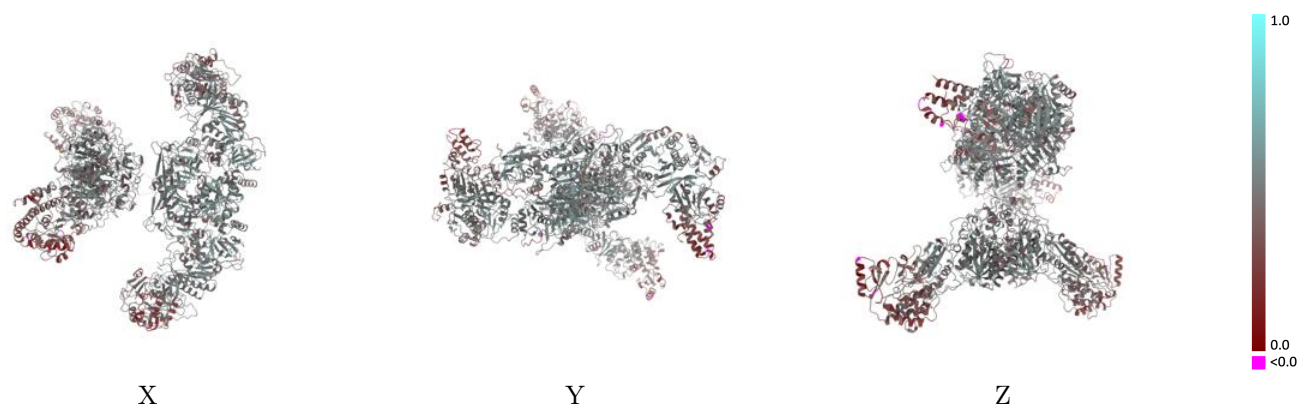
Y



Z

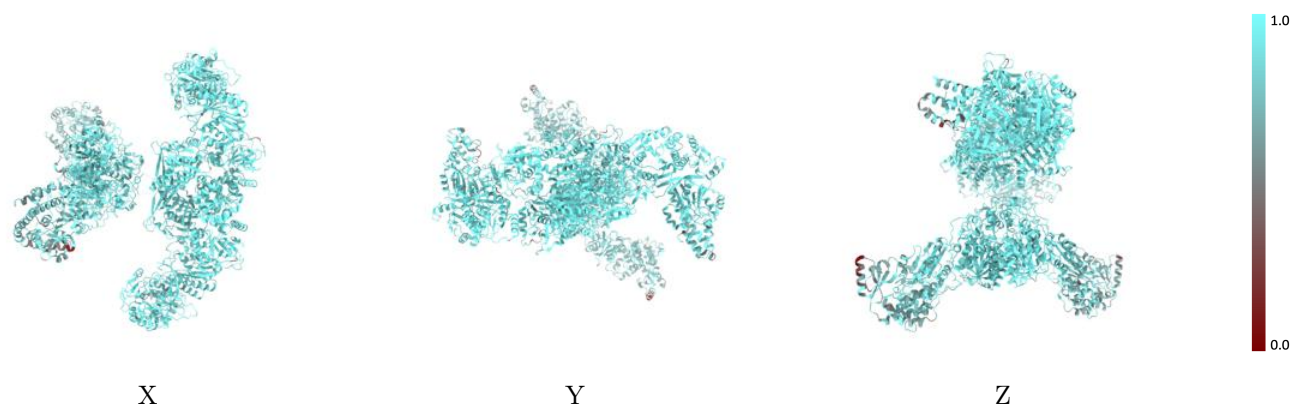
The images above show the 3D surface view of the map at the recommended contour level 0.161 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

## 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.

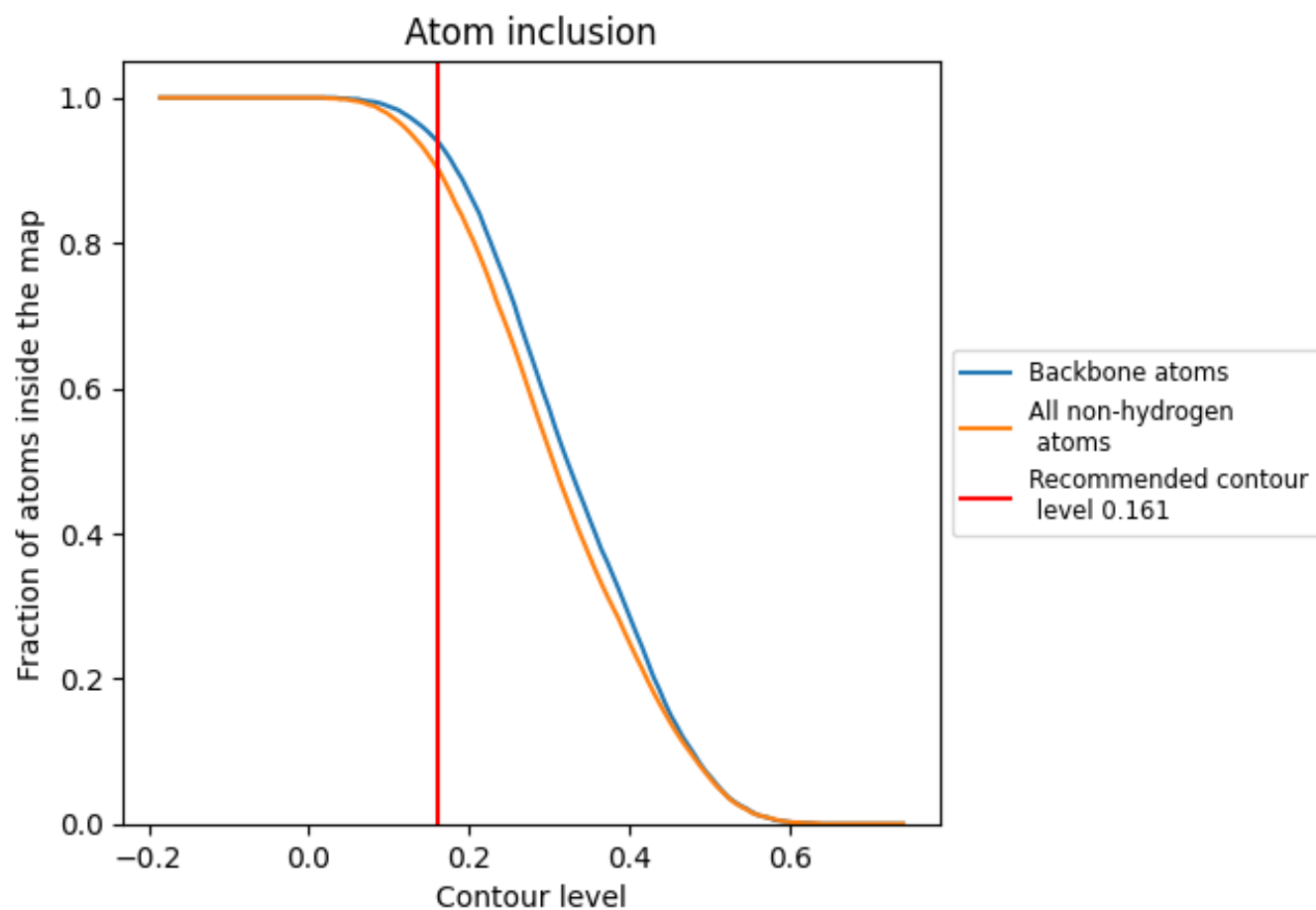
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.161).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 90% 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 (0.161) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9020	<div></div> 0.4520
A	<div></div> 0.9050	<div></div> 0.4530
B	<div></div> 0.9040	<div></div> 0.4510

