



## Full wwPDB EM Validation Report ⓘ

Feb 22, 2025 – 04:36 PM EST

PDB ID : 8VMD  
EMDB ID : EMD-43356  
Title : Modifying portion of human FASN with NADP<sup>+</sup> and the ACP at the DH domain  
Authors : Schultz, K.; Marmorstein, R.  
Deposited on : 2024-01-13  
Resolution : 3.46 Å(reported)  
Based on initial model : 8VLE

This is a Full wwPDB EM Validation 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

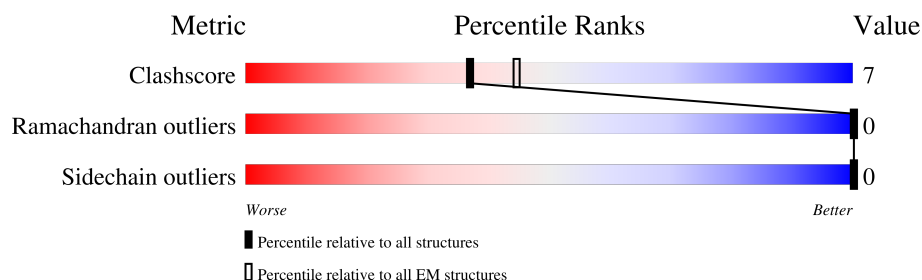
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*



The reported resolution of this entry is 3.46 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	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
1	4HH	B	2156	-	-	X	-

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 38679 atoms, of which 19335 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	1216	Total	C	H	N	O	S	0	0
			18704	5928	9358	1644	1735	39		
1	B	1289	Total	C	H	N	O	P	S	0
			19891	6290	9955	1750	1854	1	41	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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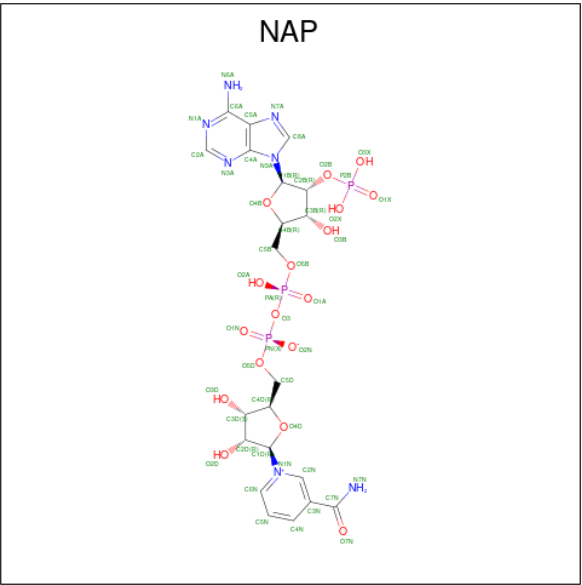
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP P49327
A	-4	MET	-	expression tag	UNP P49327
A	-3	GLY	-	expression tag	UNP P49327
A	-2	SER	-	expression tag	UNP P49327
A	-1	GLY	-	expression tag	UNP P49327
A	0	ILE	-	expression tag	UNP P49327
A	1	PRO	-	expression tag	UNP P49327
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

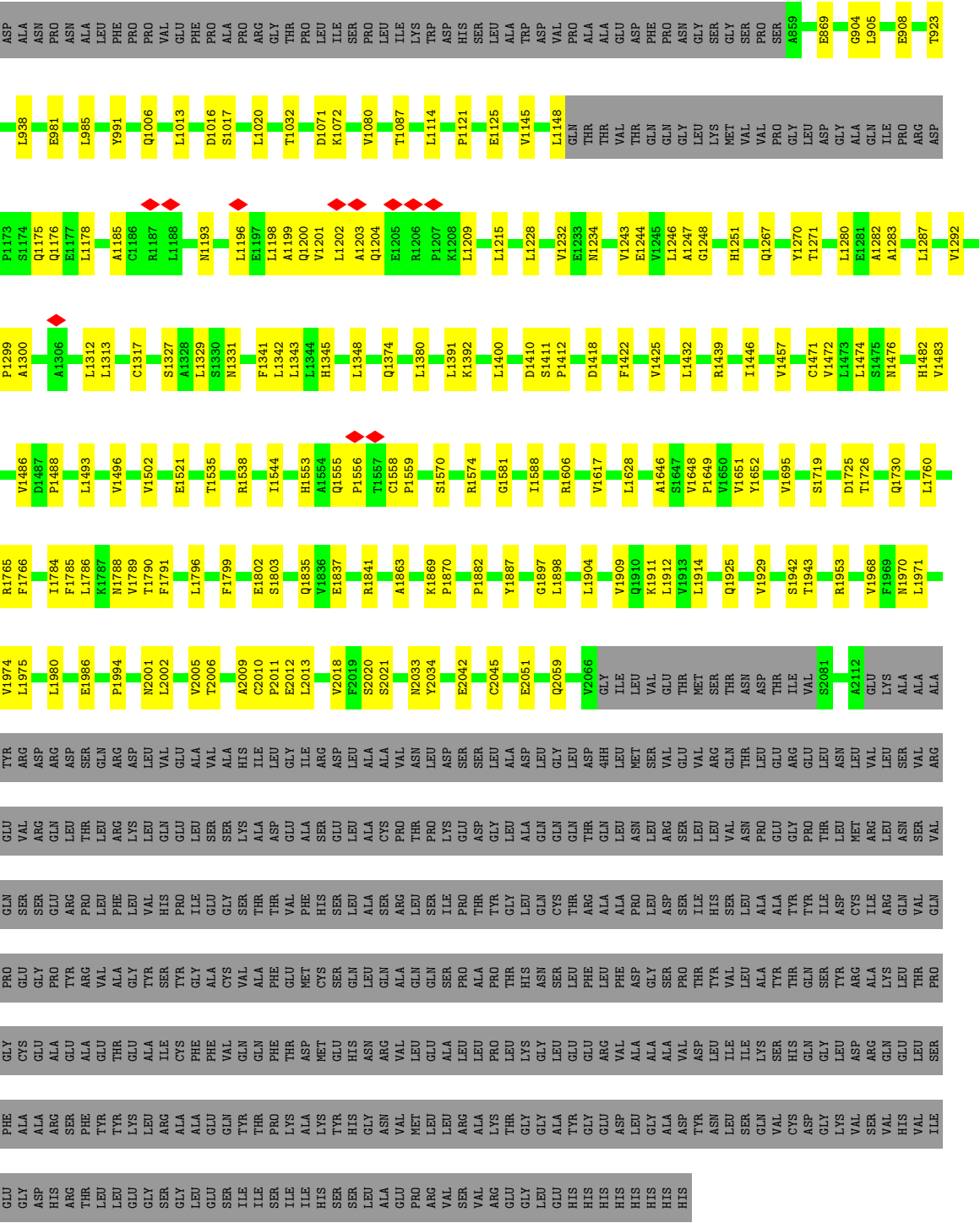
- Molecule 2 is NADP NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NAP) (formula:  $C_{21}H_{28}N_7O_{17}P_3$ ) (labeled as "Ligand of Interest" by depositor).



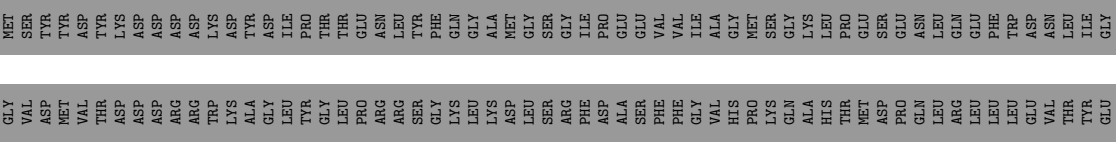
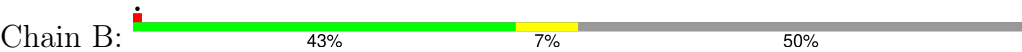
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Mol	Chain	Residues	Atoms						AltConf
2	B	1	Total	C	H	N	O	P	0
			42	10	11	5	13	3	





● Molecule 1: Fatty acid synthase







VAL	LEU	ALA	SER	ILE	LVS	GLN	D1990	A1561
	ARG	LEU	PRO	PRO	GLU	R2125	Q1562	
SER	ALA	LEU	ALA	THR	ASP	D2126	P1994	
GLU	LYS	PRO	PRO	GLY	GLY	L2127	V1566	
GLY	GLY	LYS	HIS	LEU	ALA	A2130	S1997	
LEU	GLY	GLY	ASN	GLN	GLN	V2131	N2001	
HIS	ALA	LEU	CYS	CYS	GLN	A2132	L2002	
HIS	TYR	GLU	LEU	THR	GLN	H2133	D2003	
HIS	GLY	GLU	PHE	ARG	THR	L2134	L1616	
HIS	GLU	ARG	LEU	ALA	LEU	L2135	E2012	
ASP	VAL	VAL	PHE	ALA	LEU	H2136	L1627	
LEU	LEU	ALA	ASP	PRO	ASN	L2137	L1628	
GLY	ALA	ALA	GLY	LEU	ARG	L2140	V1650	
HIS	ALA	ALA	SER	ASP	SER	L2143	N2033	
ASP	VAL	VAL	PRO	SER	LEU	Y2034	Y2034	
TYR	TYR	ASP	THR	ILE	LEU	V2143	E2042	
ASN	ASN	LEU	TYR	HIS	LEU	L2149	L1659	
LEU	ILE	ILE	VAL	SER	VAL	L2149	R1664	
SER	SER	ILE	LEU	LEU	ASN	L2152	R2048	
GLN	GLN	LYS	LEU	ALA	PRO	Q2153	R2049	
VAL	VAL	SER	TYR	ALA	GLU	D2153	Q1730	
CYS	HIS	HIS	THR	TYR	GLY	L2154	L1774	
ASP	GLN	GLN	GLN	TYR	PRO	D2155	Q2059	
GLY	GLY	LEU	SER	ILE	THR	4H2156	I2063	
LYS	LYS	LEU	TYR	ASP	THR	L2157	V1794	
VAL	VAL	ASP	ARG	CYS	MET	L2157	L1795	
SER	SER	ARG	ALA	ILE	ARG	V2162	V2056	
GLN	GLN	GLN	LYS	ARG	LEU	ILE	GLY	
GLU	GLU	GLU	LEU	GLN	ASN	T2165	LEU	
THR	THR	LEU	THR	VAL	SER	L2166	VAL	
LEU	LEU	SER	PRO	GLN	VAL	E2167	GLU	
LEU	GLU	PHE	GLY	PRO	GLN	R2168	THR	
LEU	ALA	ALA	CYS	GLU	SER	E2169	MET	
ASP	ALA	ALA	GLU	GLY	SER	SER	SER	
HIS	HIS	ARG	ALA	PRO	GLU	V2173	I1876	
ARG	ARG	SER	GLU	TYR	ARG	L2174	ASN	
THR	THR	PHE	ALA	ARG	PRO	S2175	ASP	
LEU	LEU	TYR	GLU	VAL	LEU	V2176	THR	
LEU	TYR	THR	THR	ALA	PHE	ILE	ILE	
GLU	LYS	GLY	GLU	GLY	LEU	V2179	VAL	
GLY	LEU	LEU	ALA	TYR	VAL	S2081	R1931	
SER	ARG	ARG	ILE	SER	HIS	L2182	Q1940	
GLY	GLY	ALA	CYS	TYR	PRO	T2183	V1941	
LEU	LEU	ALA	PHE	GLY	ILE	L2184	V1941	
GLU	GLU	GLU	PHE	ALA	GLU	H2103	H2103	
SER	SER	GLN	VAL	CYS	GLY	L2187	I1956	
ILE	TYR	THR	GLN	VAL	SER	ASP	A1957	
ILE	ILE	THR	GLN	ALA	THR	E2194	E1958	
SER	SER	PRO	PHE	PHE	THR	LVS	V1965	
ILE	ILE	LYS	THR	GLU	VAL	E2113	L1971	
ILE	ILE	ALA	ASP	MET	PHE	ALA	ALA	
HIS	HIS	LYS	MET	CYS	HIS	ALA	ALA	
SER	SER	TYR	GLU	SER	SER	GLU	ALA	
LEU	LEU	HIS	GLN	GLN	LEU	TYR	TYR	
GLY	GLY	GLY	ASN	ALA	ALA	ARG	ARG	
ALA	ALA	ASN	ARG	GLN	CYS	ASP	ASP	
GLU	GLU	VAL	VAL	ALA	PRO	ARG	E1981	
PRO	PRO	VAL	LEU	GLN	THR	ASP	ASP	
ARG	ARG	LEU	GLU	GLN	SER	PRO	E1986	

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	175733	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 ( $e^-/\text{\AA}^2$ )	52.474	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	1.368	Depositor
Minimum map value	-0.264	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.040	Depositor
Recommended contour level	0.265	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: NAP, 4HH

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	0.30	0/9552	0.52	0/12985
1	B	0.27	0/10114	0.49	0/13741
All	All	0.29	0/19666	0.51	0/26726

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	9346	9358	9351	142	0
1	B	9936	9955	9971	147	0
2	A	31	11	11	0	0
2	B	31	11	11	1	0
All	All	19344	19335	19344	285	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 7.

All (285) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1788:ASN:O	1:A:1789:VAL:HG23	1.76	0.85
1:B:1429:LYS:NZ	1:B:1981:GLU:O	2.10	0.85
1:B:2152:LEU:HD11	1:B:2184:LEU:HD11	1.61	0.81
1:A:1784:ILE:HD11	1:A:1785:PHE:CE1	2.15	0.81
1:B:2156:4HH:HJ3	1:B:2157:LEU:CD1	2.13	0.78
1:A:1185:ALA:O	1:A:1193:ASN:ND2	2.19	0.76
1:B:1130:GLU:N	1:B:1130:GLU:OE1	2.18	0.76
1:B:1552:ARG:O	1:B:1555:GLN:NE2	2.18	0.76
1:B:2131:VAL:HG21	1:B:2187:LEU:HD13	1.66	0.76
1:B:1965:VAL:N	1:B:2012:GLU:OE2	2.20	0.75
1:B:2143:VAL:HG21	1:B:2152:LEU:HD21	1.70	0.74
1:A:2011:PRO:HG2	1:A:2012:GLU:OE1	1.88	0.73
1:A:2051:GLU:N	1:A:2051:GLU:OE1	2.22	0.72
1:A:908:GLU:OE1	1:A:908:GLU:N	2.23	0.71
1:B:2049:ARG:NH1	1:B:2103:HIS:O	2.23	0.71
1:A:1574:ARG:HE	1:A:1588:ILE:HD12	1.55	0.70
1:B:1997:SER:O	1:B:2001:ASN:ND2	2.23	0.70
1:A:1788:ASN:O	1:A:1789:VAL:CG2	2.40	0.70
1:B:1520:GLU:N	1:B:1520:GLU:OE1	2.25	0.69
1:A:1418:ASP:OD2	1:A:1446:ILE:N	2.25	0.69
1:A:1538:ARG:NH2	1:A:1581:GLY:O	2.25	0.69
1:A:1374:GLN:OE1	1:A:1374:GLN:N	2.25	0.69
1:A:869:GLU:N	1:A:869:GLU:OE1	2.26	0.68
1:B:1492:GLU:OE1	1:B:1492:GLU:N	2.26	0.68
1:B:2156:4HH:HJ3	1:B:2157:LEU:HD11	1.75	0.68
1:B:2149:LEU:HB3	1:B:2154:LEU:HD21	1.76	0.68
1:B:2174:LEU:HD23	1:B:2179:VAL:HG12	1.75	0.68
1:A:1486:VAL:O	1:A:1493:LEU:HD22	1.94	0.68
1:B:1125:GLU:N	1:B:1125:GLU:OE1	2.26	0.67
1:A:1521:GLU:N	1:A:1521:GLU:OE1	2.27	0.67
1:A:1970:ASN:HB3	1:A:2018:VAL:HG12	1.75	0.67
1:B:2156:4HH:HL22	1:B:2157:LEU:HD21	1.76	0.67
1:B:1994:PRO:HB3	2:B:2601:NAP:H61A	1.60	0.66
1:A:1248:GLY:HA2	1:A:1280:LEU:HD13	1.78	0.65
1:B:1418:ASP:OD2	1:B:1447:ASN:N	2.29	0.65
1:B:1835:GLN:N	1:B:1835:GLN:OE1	2.30	0.65
1:A:1071:ASP:OD1	1:A:1072:LYS:N	2.30	0.65
1:A:1457:VAL:HG11	1:A:1471:CYS:HB2	1.79	0.65
1:A:2042:GLU:OE2	1:A:2059:GLN:NE2	2.29	0.65
1:B:1177:GLU:N	1:B:1177:GLU:OE1	2.29	0.65
1:A:1802:GLU:HG3	1:A:1803:SER:N	2.12	0.64
1:A:1267:GLN:OE1	1:A:1267:GLN:N	2.30	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1145:VAL:HG21	1:B:1356:ILE:HG12	1.79	0.63
1:A:1198:LEU:HD12	1:A:1199:ALA:N	2.14	0.63
1:B:1214:LEU:O	1:B:1396:TYR:OH	2.07	0.62
1:A:1835:GLN:N	1:A:1835:GLN:OE1	2.32	0.62
1:A:1121:PRO:O	1:A:1392:LYS:NZ	2.32	0.62
1:A:1488:PRO:HA	1:A:1493:LEU:HD23	1.79	0.62
1:B:1437:SER:O	1:B:1468:ARG:NH1	2.32	0.62
1:A:1558:CYS:HB2	1:A:1559:PRO:CD	2.30	0.61
1:A:1765:ARG:HG2	1:A:1790:THR:HG22	1.83	0.61
1:A:1986:GLU:N	1:A:1986:GLU:OE1	2.32	0.61
1:A:1410:ASP:OD1	1:A:1411:SER:N	2.34	0.60
1:B:1120:THR:HG21	1:B:1517:PHE:CZ	2.37	0.60
1:B:1349:ARG:NH2	1:B:1371:ILE:O	2.35	0.60
1:B:2176:VAL:O	1:B:2179:VAL:HG22	2.01	0.60
1:B:2182:LEU:HD21	1:B:2187:LEU:HD21	1.83	0.60
1:A:1125:GLU:N	1:A:1125:GLU:OE1	2.35	0.59
1:A:1784:ILE:HD11	1:A:1785:PHE:CD1	2.36	0.59
1:A:2018:VAL:CG2	1:A:2045:CYS:SG	2.91	0.59
1:B:1794:VAL:C	1:B:1795:LEU:HD12	2.23	0.59
1:A:981:GLU:OE1	1:A:981:GLU:N	2.35	0.59
1:B:1986:GLU:OE1	1:B:1986:GLU:N	2.35	0.59
1:A:1887:TYR:CD2	1:A:1909:VAL:HG13	2.39	0.58
1:B:2149:LEU:CD1	1:B:2182:LEU:HD23	2.34	0.58
1:A:1617:VAL:CG1	1:A:1628:LEU:HD23	2.34	0.58
1:A:1725:ASP:OD1	1:A:1726:THR:N	2.37	0.57
1:B:1562:GLN:O	1:B:1627:LEU:HD12	2.04	0.57
1:A:1176:GLN:N	1:A:1176:GLN:OE1	2.37	0.57
1:B:2063:ILE:N	1:B:2063:ILE:HD12	2.20	0.57
1:B:1366:GLN:OE1	1:B:1369:GLN:NE2	2.38	0.57
1:A:1175:GLN:OE1	1:A:1175:GLN:N	2.37	0.56
1:B:1458:ASN:ND2	1:B:2025:GLY:O	2.38	0.56
1:A:1909:VAL:HG12	1:A:1911:LYS:H	1.69	0.56
1:A:1016:ASP:OD1	1:A:1017:SER:N	2.38	0.56
1:B:1730:GLN:N	1:B:1730:GLN:OE1	2.35	0.56
1:B:1561:ALA:HB1	1:B:1627:LEU:HD11	1.88	0.56
1:A:1312:LEU:HD12	1:A:1341:PHE:O	2.06	0.56
1:B:1206:ARG:CZ	1:B:1209:LEU:HD22	2.36	0.56
1:B:1457:VAL:HG21	1:B:1471:CYS:HB3	1.87	0.56
1:B:1244:GLU:HG2	1:B:1314:VAL:HG23	1.87	0.55
1:B:2167:GLU:HG3	1:B:2173:VAL:HG22	1.87	0.55
1:B:1102:ALA:HB2	1:B:2156:4HH:HL12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2042:GLU:OE2	1:B:2059:GLN:NE2	2.39	0.55
1:B:2149:LEU:HD21	1:B:2187:LEU:CD1	2.36	0.55
1:A:1555:GLN:N	1:A:1556:PRO:CD	2.70	0.55
1:B:2033:ASN:OD1	1:B:2034:TYR:N	2.40	0.55
1:A:1244:GLU:OE1	1:A:1270:TYR:OH	2.24	0.55
1:B:869:GLU:N	1:B:869:GLU:OE1	2.40	0.55
1:B:1120:THR:HG21	1:B:1517:PHE:HZ	1.71	0.55
1:A:1243:VAL:HG12	1:A:1271:THR:CG2	2.37	0.54
1:A:1784:ILE:CD1	1:A:1785:PHE:CD1	2.90	0.54
1:B:1249:HIS:O	1:B:1251:HIS:ND1	2.40	0.54
1:B:2149:LEU:HD11	1:B:2182:LEU:HD23	1.90	0.54
1:B:1274:ASP:OD1	1:B:1275:ARG:N	2.40	0.54
1:B:1317:CYS:N	1:B:1345:HIS:O	2.41	0.53
1:B:1338:GLU:HG2	1:B:1407:THR:HG22	1.89	0.53
1:B:888:ALA:HB2	1:B:2156:4HH:HS3	1.91	0.53
1:B:2143:VAL:HG21	1:B:2152:LEU:CD2	2.37	0.53
1:A:1471:CYS:SG	1:A:1472:VAL:N	2.82	0.53
1:A:1570:SER:OG	1:A:1646:ALA:O	2.20	0.53
1:B:862:TYR:HH	1:B:898:THR:HG1	1.53	0.53
1:A:1558:CYS:HB2	1:A:1559:PRO:HD2	1.89	0.53
1:A:1975:LEU:HD12	1:A:1975:LEU:O	2.08	0.53
1:B:2134:ILE:HG21	1:B:2162:VAL:HG23	1.91	0.53
1:B:1181:LEU:HD23	1:B:1360:LEU:HD21	1.90	0.53
1:B:1928:GLN:OE1	1:B:1931:ARG:NH2	2.42	0.53
1:A:1411:SER:OG	1:A:1439:ARG:NH2	2.42	0.53
1:A:2002:LEU:O	1:A:2006:THR:HG23	2.09	0.53
1:B:1188:LEU:HD13	1:B:1197:GLU:HG2	1.90	0.53
1:B:1417:VAL:HG12	1:B:1417:VAL:O	2.09	0.53
1:B:1418:ASP:OD2	1:B:1446:ILE:N	2.40	0.53
1:A:1248:GLY:O	1:A:1251:HIS:NE2	2.40	0.52
1:B:1052:VAL:HG11	1:B:1055:ILE:HD11	1.91	0.52
1:B:1379:SER:O	1:B:1382:SER:OG	2.23	0.52
1:B:1521:GLU:OE1	1:B:1521:GLU:N	2.36	0.52
1:A:1553:HIS:HB3	1:A:1555:GLN:HE21	1.74	0.52
1:B:1103:PRO:HB2	1:B:2155:ASP:OD2	2.08	0.52
1:A:1343:LEU:HD21	1:A:1400:LEU:HD11	1.91	0.52
1:A:2018:VAL:HG21	1:A:2045:CYS:SG	2.49	0.52
1:A:1246:LEU:HD11	1:A:1299:PRO:HG2	1.91	0.52
1:A:2033:ASN:OD1	1:A:2034:TYR:N	2.43	0.52
1:A:1327:SER:O	1:A:1331:ASN:ND2	2.43	0.51
1:A:1446:ILE:HG21	1:A:1486:VAL:HG21	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:904:GLY:C	1:B:905:LEU:HD22	2.31	0.51
1:B:2137:ILE:HD11	1:B:2152:LEU:HD22	1.92	0.51
1:B:2156:4HH:CL2	1:B:2157:LEU:HD21	2.41	0.51
1:A:1476:ASN:ND2	1:A:1482:HIS:O	2.43	0.51
1:A:1786:LEU:HG	1:B:1774:LEU:HB3	1.91	0.51
1:B:2149:LEU:HD11	1:B:2187:LEU:HD11	1.93	0.51
1:A:1287:LEU:HG	1:A:1292:VAL:HG21	1.93	0.51
1:A:1788:ASN:C	1:A:1789:VAL:HG23	2.30	0.51
1:B:2003:ASP:OD1	1:B:2048:ARG:NH1	2.44	0.51
1:B:1493:LEU:HA	1:B:1496:VAL:HG12	1.93	0.51
1:A:1248:GLY:HA2	1:A:1280:LEU:HB2	1.94	0.50
1:A:1412:PRO:O	1:A:1439:ARG:NH2	2.44	0.50
1:A:1726:THR:O	1:A:1726:THR:HG22	2.10	0.50
1:A:1299:PRO:O	1:A:1331:ASN:ND2	2.42	0.50
1:B:2149:LEU:HB2	1:B:2154:LEU:HD11	1.92	0.50
1:B:1029:PHE:O	1:B:1032:THR:OG1	2.23	0.50
1:B:1616:LEU:CD1	1:B:1650:VAL:HG22	2.41	0.50
1:A:1020:LEU:HD22	1:A:1032:THR:CG2	2.41	0.50
1:B:1185:ALA:HB1	1:B:1190:LEU:HD21	1.94	0.50
1:B:952:LEU:HD12	1:B:952:LEU:O	2.12	0.50
1:B:1141:CYS:O	1:B:1145:VAL:HG23	2.12	0.50
1:B:2137:ILE:CD1	1:B:2152:LEU:HD22	2.43	0.49
1:A:1209:LEU:O	1:A:1215:LEU:HD22	2.12	0.49
1:B:1246:LEU:N	1:B:1246:LEU:HD12	2.28	0.49
1:B:1453:VAL:O	1:B:1457:VAL:HG23	2.13	0.49
1:B:2152:LEU:HD11	1:B:2184:LEU:CD1	2.39	0.49
1:B:1134:LEU:HD12	1:B:1214:LEU:HD23	1.95	0.49
1:A:1432:LEU:HD12	1:A:1980:LEU:HD23	1.94	0.48
1:A:1555:GLN:HG3	1:A:1882:PRO:HA	1.95	0.48
1:B:2130:ALA:O	1:B:2133:HIS:ND1	2.46	0.48
1:A:2010:CYS:HB3	1:A:2013:LEU:HB2	1.95	0.48
1:A:985:LEU:CD1	1:A:1013:LEU:HD23	2.43	0.48
1:A:1329:LEU:HD12	1:A:1380:LEU:HG	1.94	0.48
1:A:1953:ARG:HA	1:A:2005:VAL:HG21	1.95	0.48
1:B:1047:TYR:OH	1:B:1586:ASP:OD2	2.21	0.48
1:A:1080:VAL:HG22	1:A:1087:THR:HG23	1.96	0.48
1:A:1887:TYR:HD2	1:A:1909:VAL:HG13	1.79	0.48
1:B:889:THR:HG21	1:B:1030:MET:CB	2.44	0.48
1:B:2086:GLN:HG2	1:B:2110:VAL:HG23	1.95	0.48
1:B:1603:PHE:CE1	1:B:1628:LEU:HD21	2.49	0.48
1:B:2140:LEU:HD11	1:B:2184:LEU:HD22	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2156:4HH:HJ3	1:B:2157:LEU:HD12	1.95	0.48
1:A:1422:PHE:O	1:A:1425:VAL:HG12	2.14	0.47
1:A:1201:VAL:HG13	1:A:1204:GLN:HB2	1.95	0.47
1:A:1282:ALA:O	1:A:1283:ALA:HB3	2.13	0.47
1:A:1553:HIS:HB2	1:A:1555:GLN:HG2	1.96	0.47
1:A:1904:LEU:HB3	1:A:1909:VAL:HG21	1.96	0.47
1:A:991:TYR:CZ	1:A:1006:GLN:HA	2.49	0.47
1:A:1483:VAL:O	1:A:1483:VAL:HG13	2.14	0.47
1:A:1788:ASN:OD1	1:B:1795:LEU:HD13	2.14	0.47
1:A:2001:ASN:O	1:A:2005:VAL:HG12	2.15	0.47
1:B:2134:ILE:HD11	1:B:2165:THR:HG21	1.96	0.47
1:B:973:GLU:OE1	1:B:973:GLU:N	2.44	0.47
1:B:2131:VAL:O	1:B:2135:LEU:HD13	2.14	0.47
1:B:1541:LEU:HD11	1:B:1840:PHE:HB3	1.96	0.47
1:A:1243:VAL:HG12	1:A:1271:THR:HG22	1.97	0.47
1:A:2006:THR:O	1:A:2010:CYS:HB2	2.15	0.47
1:A:2020:SER:OG	1:A:2021:SER:N	2.47	0.47
1:A:1606:ARG:NH1	1:A:1863:ALA:O	2.46	0.47
1:A:2018:VAL:HG22	1:A:2045:CYS:SG	2.54	0.47
1:A:1802:GLU:CG	1:A:1803:SER:N	2.76	0.47
1:B:1417:VAL:N	1:B:1444:LYS:O	2.47	0.47
1:B:1348:LEU:HD21	1:B:1399:THR:HG21	1.97	0.46
1:B:1448:CYS:SG	1:B:1451:SER:N	2.88	0.46
1:A:1766:PHE:CD1	1:A:1791:PHE:CE1	3.04	0.46
1:A:1974:VAL:O	1:A:1974:VAL:HG13	2.15	0.46
1:B:1976:ARG:NH1	1:B:1990:ASP:OD2	2.49	0.46
1:B:1144:LEU:HD13	1:B:1182:LEU:HB2	1.98	0.46
1:B:1302:PRO:HA	1:B:1331:ASN:HB3	1.97	0.46
1:A:1493:LEU:HA	1:A:1496:VAL:HG22	1.97	0.46
1:B:1566:VAL:HG13	1:B:1603:PHE:HB2	1.97	0.46
1:A:1317:CYS:N	1:A:1345:HIS:O	2.49	0.45
1:B:939:GLU:OE1	1:B:939:GLU:N	2.47	0.45
1:A:1020:LEU:HD22	1:A:1032:THR:HG22	1.97	0.45
1:A:1914:LEU:HD12	1:A:1914:LEU:N	2.32	0.45
1:B:1940:GLN:NE2	1:B:1958:GLU:OE2	2.48	0.45
1:A:1145:VAL:HG12	1:A:1145:VAL:O	2.17	0.45
1:A:1898:LEU:HD11	1:A:1925:GLN:HG2	1.99	0.45
1:A:1802:GLU:HG3	1:A:1803:SER:H	1.80	0.45
1:A:1247:ALA:C	1:A:1280:LEU:HD22	2.37	0.45
1:A:1695:VAL:O	1:A:1719:SER:OG	2.30	0.45
1:B:1346:THR:O	1:B:1399:THR:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1313:LEU:HB2	1:A:1342:LEU:HD13	1.99	0.44
1:B:1197:GLU:OE1	1:B:1197:GLU:N	2.44	0.44
1:A:1246:LEU:HD12	1:A:1246:LEU:N	2.32	0.44
1:B:885:LEU:HD22	1:B:922:ALA:HB1	1.99	0.44
1:B:1146:GLN:OE1	1:B:1149:GLN:NE2	2.51	0.44
1:A:1391:LEU:HD23	1:A:1391:LEU:C	2.38	0.44
1:A:1651:VAL:HG23	1:A:1652:TYR:N	2.33	0.44
1:A:1837:GLU:OE2	1:A:1841:ARG:NH2	2.50	0.44
1:B:1545:ARG:HG2	1:B:1876:ILE:HD11	1.98	0.44
1:A:1942:SER:O	1:A:1943:THR:OG1	2.22	0.44
1:A:1974:VAL:HG12	1:A:1994:PRO:HG3	1.99	0.44
1:B:2149:LEU:HD12	1:B:2182:LEU:HD23	1.99	0.44
1:A:1196:LEU:O	1:A:1200:GLN:N	2.48	0.44
1:B:2127:LEU:HD12	1:B:2127:LEU:H	1.83	0.44
1:A:938:LEU:HD21	1:B:945:GLU:HB2	1.99	0.44
1:A:1202:LEU:HD12	1:A:1202:LEU:C	2.38	0.44
1:B:2156:4HH:HL22	1:B:2157:LEU:HD11	2.00	0.44
1:B:1300:ALA:O	1:B:1331:ASN:OD1	2.35	0.44
1:B:1888:ILE:CD1	1:B:1956:ILE:HD13	2.48	0.44
1:A:1925:GLN:O	1:A:1929:VAL:HG23	2.18	0.43
1:A:1968:VAL:O	1:A:1968:VAL:HG23	2.18	0.43
1:A:1760:LEU:HD11	1:A:1766:PHE:HB2	2.00	0.43
1:B:1555:GLN:OE1	1:B:1555:GLN:N	2.47	0.43
1:B:924:ILE:HD12	1:B:924:ILE:N	2.33	0.43
1:B:909:GLN:N	1:B:909:GLN:OE1	2.50	0.43
1:B:2149:LEU:CB	1:B:2154:LEU:HD11	2.49	0.43
1:A:1202:LEU:O	1:A:1203:ALA:HB3	2.18	0.43
1:B:879:THR:OG1	1:B:1000:ASP:O	2.35	0.43
1:B:997:ARG:NH2	1:B:1043:LYS:O	2.50	0.43
1:B:1122:HIS:ND1	1:B:1511:TRP:O	2.51	0.43
1:B:1659:LEU:O	1:B:1664:ARG:N	2.51	0.43
1:A:1786:LEU:HD21	1:B:1774:LEU:HB2	2.00	0.43
1:A:1348:LEU:HD22	1:A:1374:GLN:HB3	2.00	0.42
1:A:1228:LEU:O	1:A:1232:VAL:HG23	2.19	0.42
1:A:1897:GLY:HA2	1:A:1971:LEU:HD22	2.00	0.42
1:B:2174:LEU:CD2	1:B:2182:LEU:HD22	2.50	0.42
1:A:905:LEU:N	1:A:905:LEU:HD12	2.34	0.42
1:A:1730:GLN:OE1	1:A:1730:GLN:N	2.48	0.42
1:B:1181:LEU:CD2	1:B:1360:LEU:HD21	2.50	0.42
1:B:1860:GLU:OE1	1:B:1860:GLU:N	2.52	0.42
1:B:862:TYR:OH	1:B:898:THR:OG1	2.27	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1195:GLN:O	1:B:1199:ALA:N	2.43	0.42
1:B:1239:LYS:NZ	1:B:1267:GLN:OE1	2.32	0.42
1:B:991:TYR:OH	1:B:1006:GLN:HA	2.20	0.42
1:B:1031:ASP:OD1	1:B:1031:ASP:O	2.38	0.42
1:B:2166:LEU:HD23	1:B:2169:GLU:OE2	2.20	0.42
1:B:1209:LEU:N	1:B:1210:PRO:HD2	2.34	0.42
1:B:1485:GLU:OE1	1:B:1485:GLU:N	2.46	0.42
1:B:1941:VAL:HG23	1:B:1941:VAL:O	2.20	0.42
1:A:1446:ILE:HG22	1:A:1474:LEU:HG	2.02	0.41
1:A:1796:LEU:HD12	1:A:1799:PHE:CD2	2.55	0.41
1:B:925:LEU:N	1:B:925:LEU:HD12	2.35	0.41
1:B:1209:LEU:HD23	1:B:1319:VAL:HG13	2.01	0.41
1:A:1114:LEU:HD12	1:A:1114:LEU:N	2.35	0.41
1:B:1031:ASP:O	1:B:1035:GLN:HG3	2.20	0.41
1:A:1178:LEU:HD23	1:A:1178:LEU:O	2.20	0.41
1:A:1148:LEU:HD12	1:A:1148:LEU:N	2.36	0.41
1:A:1912:LEU:HD23	1:A:1914:LEU:HD11	2.03	0.41
1:B:1971:LEU:N	1:B:1971:LEU:HD12	2.36	0.41
1:A:1446:ILE:HG21	1:A:1486:VAL:CG2	2.51	0.41
1:A:1446:ILE:HD12	1:A:1446:ILE:C	2.42	0.41
1:A:1234:ASN:OD1	1:A:1502:VAL:N	2.38	0.41
1:A:1300:ALA:O	1:A:1331:ASN:ND2	2.54	0.41
1:A:1446:ILE:HG22	1:A:1474:LEU:CD1	2.51	0.41
1:A:1535:THR:HG22	1:A:1544:ILE:HG12	2.02	0.41
1:A:1628:LEU:HD12	1:A:1628:LEU:O	2.20	0.41
1:A:1869:LYS:NZ	1:A:1870:PRO:O	2.53	0.41
1:A:2005:VAL:O	1:A:2009:ALA:HB3	2.21	0.41
1:B:2132:ALA:HB2	1:B:2140:LEU:HD22	2.02	0.41
1:B:2153:GLY:O	1:B:2154:LEU:HD23	2.21	0.41
1:A:1648:VAL:N	1:A:1649:PRO:CD	2.84	0.40
1:B:991:TYR:CZ	1:B:1006:GLN:HA	2.57	0.40
1:A:904:GLY:C	1:A:905:LEU:HD12	2.42	0.40
1:A:923:THR:O	1:A:923:THR:HG23	2.22	0.40
1:B:1049:PRO:O	1:B:2156:4HH:HO2	2.22	0.40
1:B:1344:LEU:HD23	1:B:1344:LEU:C	2.41	0.40
1:B:1443:LEU:N	1:B:1470:ARG:O	2.54	0.40
1:B:2132:ALA:HB2	1:B:2140:LEU:HD13	2.03	0.40
1:A:1343:LEU:C	1:A:1343:LEU:HD23	2.42	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1210/2553 (47%)	1162 (96%)	48 (4%)	0	100	100
1	B	1280/2553 (50%)	1233 (96%)	47 (4%)	0	100	100
All	All	2490/5106 (49%)	2395 (96%)	95 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1009/2116 (48%)	1009 (100%)	0	100	100
1	B	1073/2116 (51%)	1073 (100%)	0	100	100
All	All	2082/4232 (49%)	2082 (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 (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1296	GLN
1	A	1504	ASN
1	A	1530	HIS
1	A	1553	HIS
1	A	1555	GLN
1	A	1763	HIS

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Mol	Chain	Res	Type
1	A	2100	ASN
1	B	1110	GLN
1	B	1369	GLN
1	B	1504	ASN
1	B	1709	GLN
1	B	1763	HIS
1	B	1845	GLN
1	B	1983	GLN
1	B	2086	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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	$\# Z  > 2$
1	4HH	B	2156	1	22,26,27	0.42	0	27,35,37	0.56	0

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
1	4HH	B	2156	1	-	22/33/35/37	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	2156	4HH	CB-OG-P-O1P
1	B	2156	4HH	CB-OG-P-O2P
1	B	2156	4HH	CB-OG-P-O3P
1	B	2156	4HH	CJ-CK-CM-CL3
1	B	2156	4HH	CJ-CK-CM-OM
1	B	2156	4HH	CL1-CK-CM-CL3
1	B	2156	4HH	CL1-CK-CM-OM
1	B	2156	4HH	CL2-CK-CM-CL3
1	B	2156	4HH	CL2-CK-CM-OM
1	B	2156	4HH	NN-CL3-CM-OM
1	B	2156	4HH	CJ-O3P-P-OG
1	B	2156	4HH	CJ-O3P-P-O1P
1	B	2156	4HH	NR-CS-CT-SU
1	B	2156	4HH	OR-CQ-NR-CS
1	B	2156	4HH	CP-CQ-NR-CS
1	B	2156	4HH	CM-CL3-NN-CO
1	B	2156	4HH	ON-CL3-CM-OM
1	B	2156	4HH	O3P-CJ-CK-CL1
1	B	2156	4HH	CJ-O3P-P-O2P
1	B	2156	4HH	ON-CL3-NN-CO
1	B	2156	4HH	O3P-CJ-CK-CL2
1	B	2156	4HH	NN-CO-CP-CQ

There are no ring outliers.

1 monomer is involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	2156	4HH	9	0

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

2 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	NAP	A	2601	-	28,33,52	0.81	0	40,52,80	1.08	2 (5%)
2	NAP	B	2601	-	28,33,52	0.82	0	40,52,80	1.04	2 (5%)

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	NAP	A	2601	-	-	6/17/37/67	0/3/3/5
2	NAP	B	2601	-	-	6/17/37/67	0/3/3/5

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2601	NAP	P2B-O2B-C2B	-4.78	110.68	123.43
2	A	2601	NAP	P2B-O2B-C2B	-4.76	110.73	123.43
2	B	2601	NAP	C5A-C6A-N6A	2.26	123.75	120.31
2	A	2601	NAP	C5A-C6A-N6A	2.13	123.56	120.31

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	2601	NAP	C5B-O5B-PA-O1A
2	A	2601	NAP	C5B-O5B-PA-O2A
2	A	2601	NAP	C5B-O5B-PA-O3
2	A	2601	NAP	C4B-C5B-O5B-PA
2	A	2601	NAP	C3B-C4B-C5B-O5B
2	B	2601	NAP	C5B-O5B-PA-O3
2	B	2601	NAP	PA-O3-PN-O2N
2	A	2601	NAP	O4B-C4B-C5B-O5B
2	B	2601	NAP	PN-O3-PA-O5B
2	B	2601	NAP	C5B-O5B-PA-O1A

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	2601	NAP	PA-O3-PN-O1N
2	B	2601	NAP	PA-O3-PN-O5D

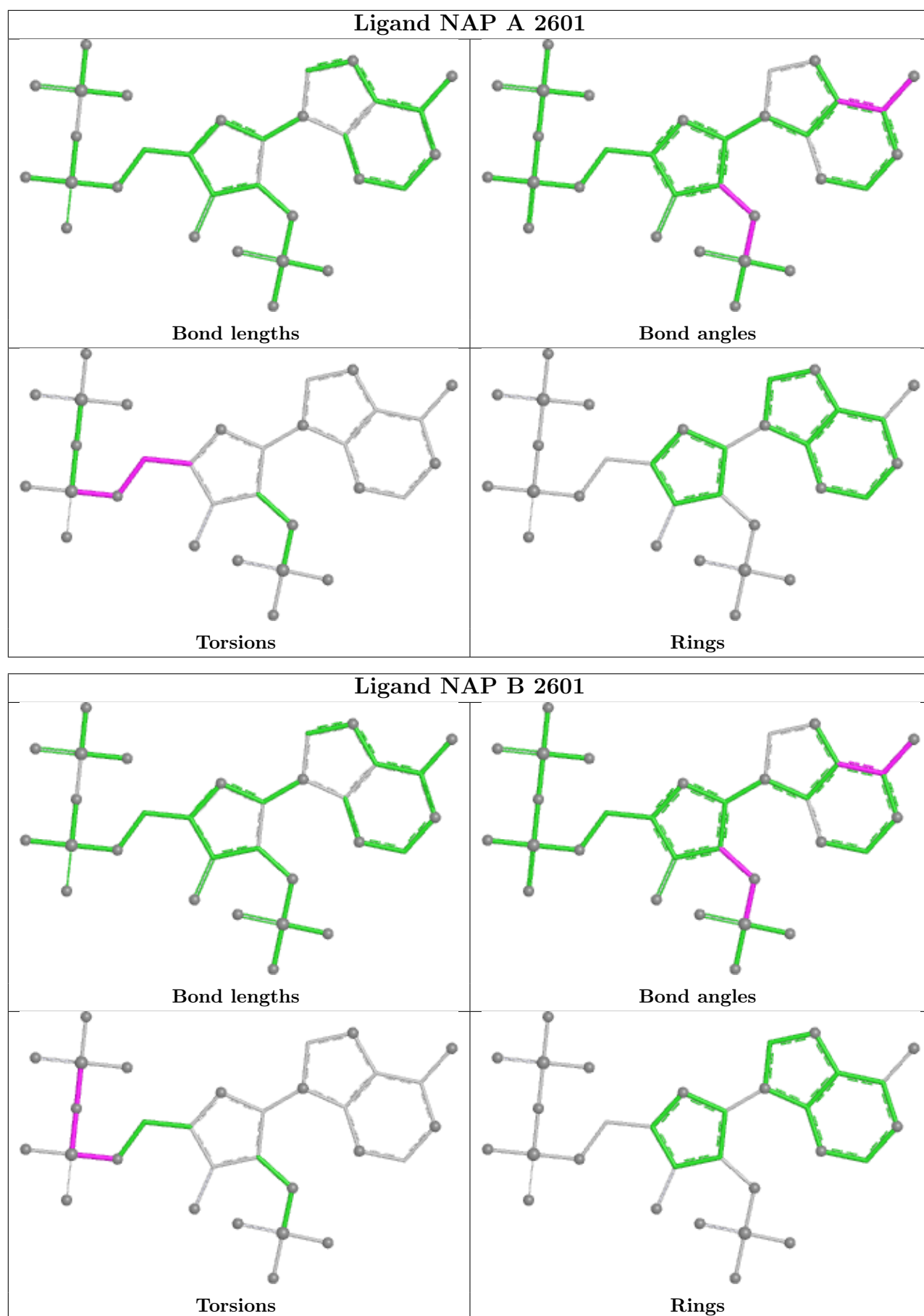
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	2601	NAP	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.

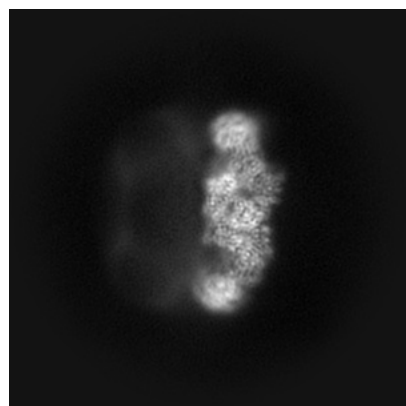
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43356. These allow visual inspection of the internal detail of the map and identification of artifacts.

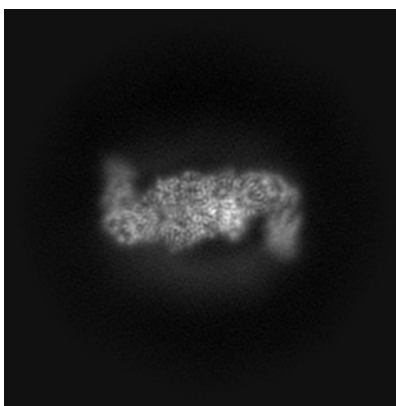
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

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

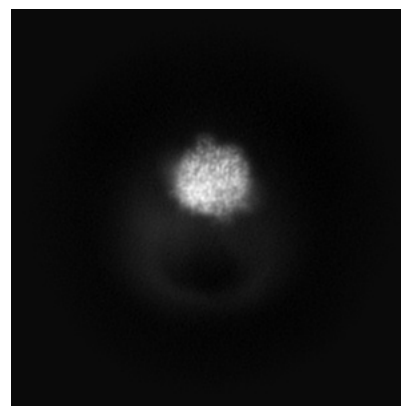
#### 6.1.1 Primary map



X

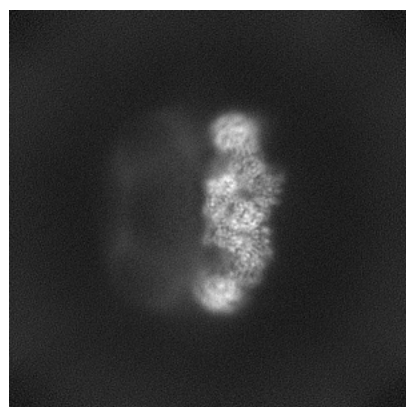


Y

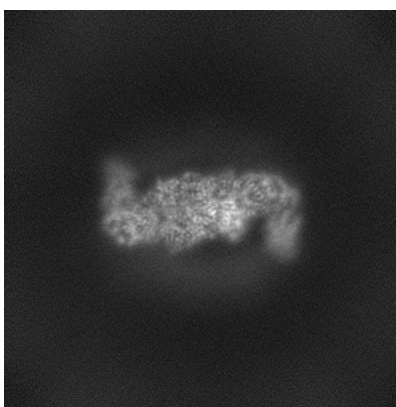


Z

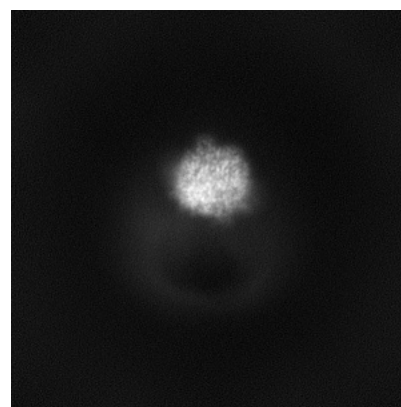
#### 6.1.2 Raw map



X



Y

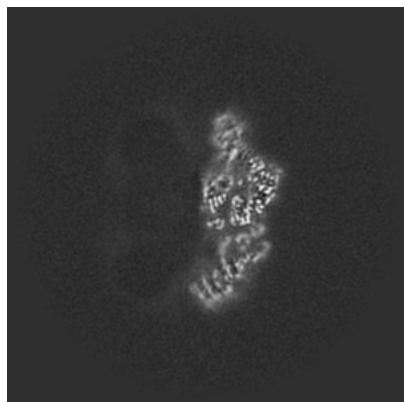


Z

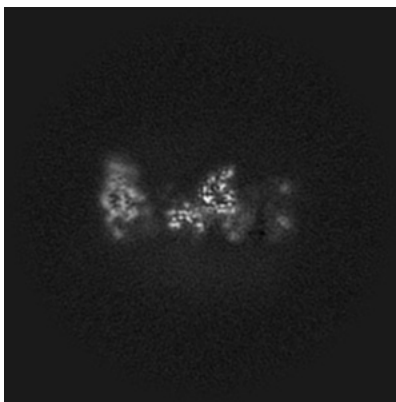
The images above show the map projected in three orthogonal directions.

## 6.2 Central slices [i](#)

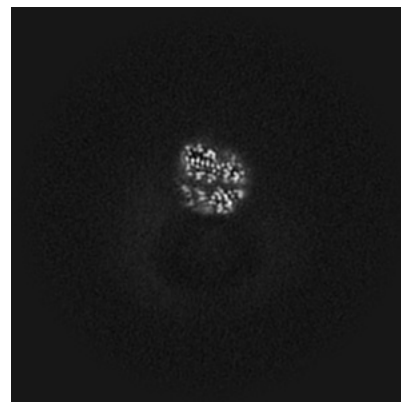
### 6.2.1 Primary map



X Index: 180

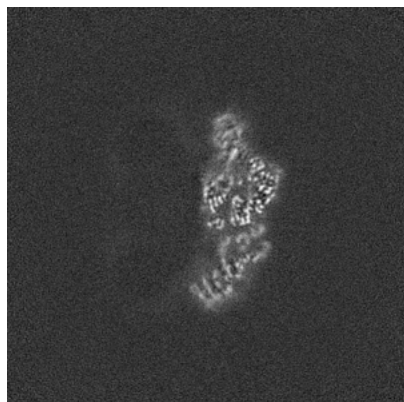


Y Index: 180

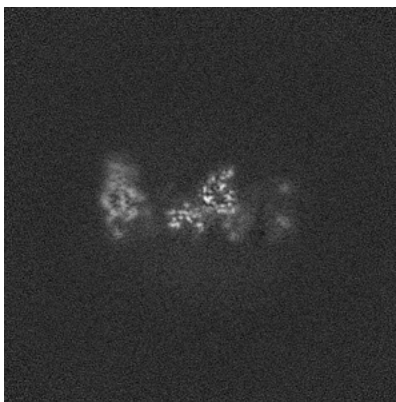


Z Index: 180

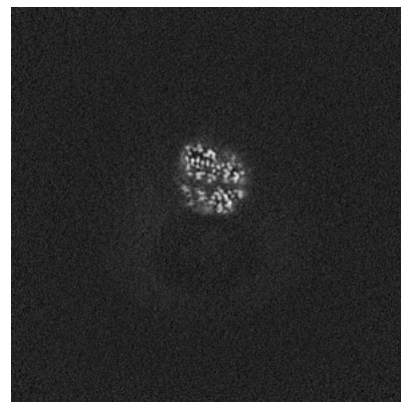
### 6.2.2 Raw map



X Index: 180



Y Index: 180

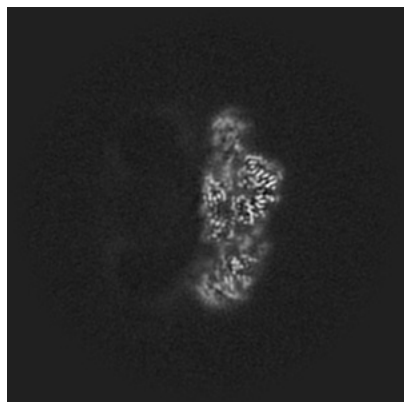


Z Index: 180

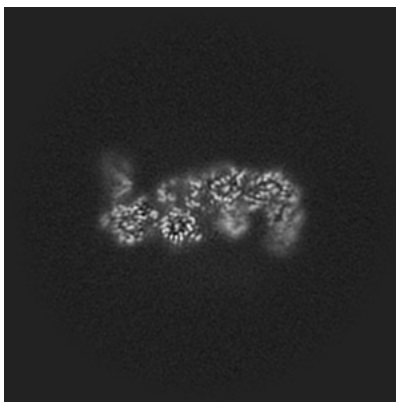
The images above show central slices of the map in three orthogonal directions.

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

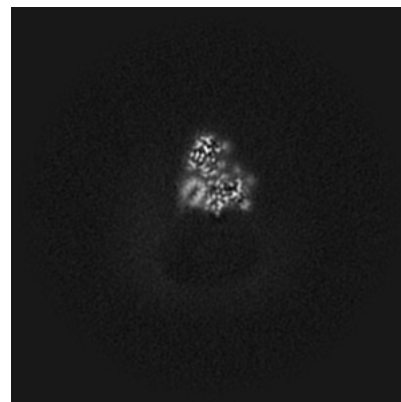
### 6.3.1 Primary map



X Index: 177

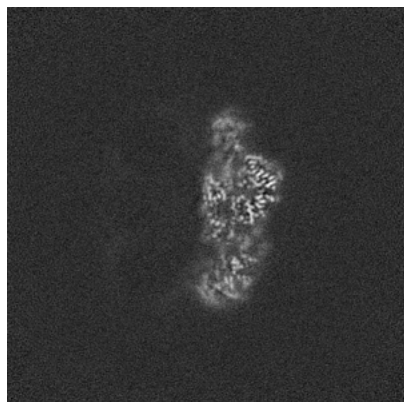


Y Index: 201

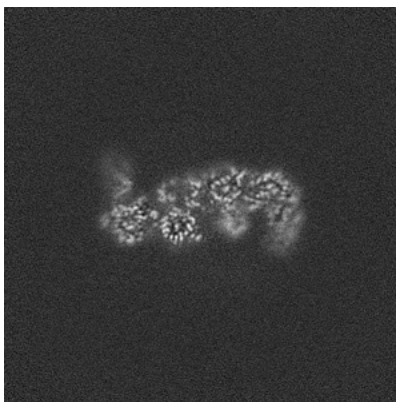


Z Index: 202

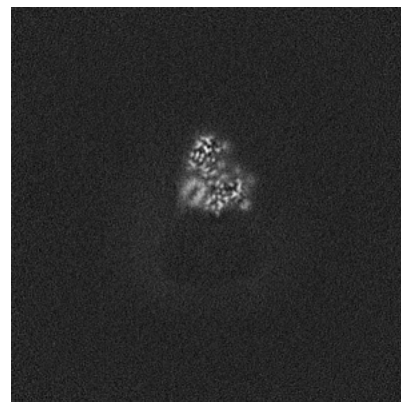
### 6.3.2 Raw map



X Index: 177



Y Index: 201

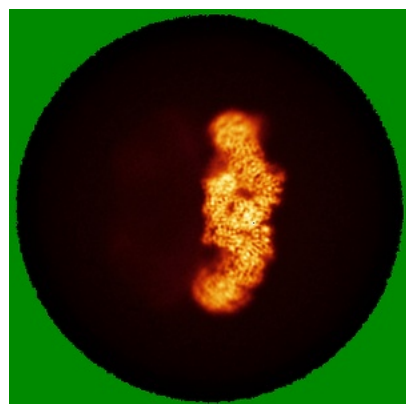


Z Index: 202

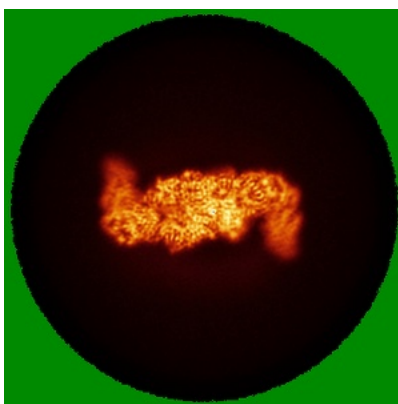
The images above show the largest variance slices of the map in three orthogonal directions.

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

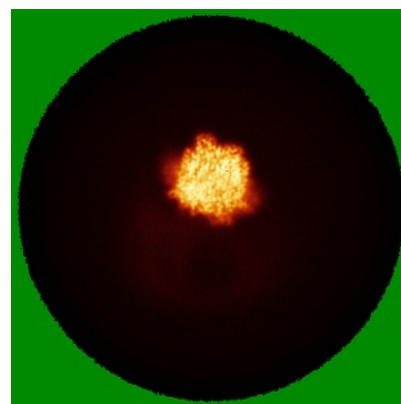
### 6.4.1 Primary map



X

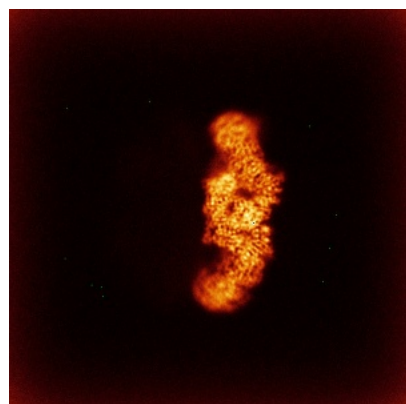


Y

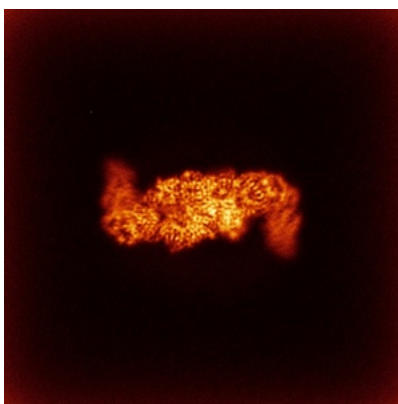


Z

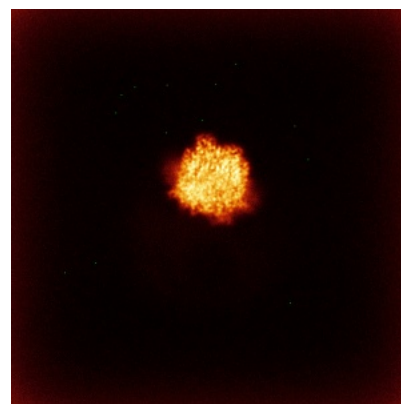
### 6.4.2 Raw map



X



Y



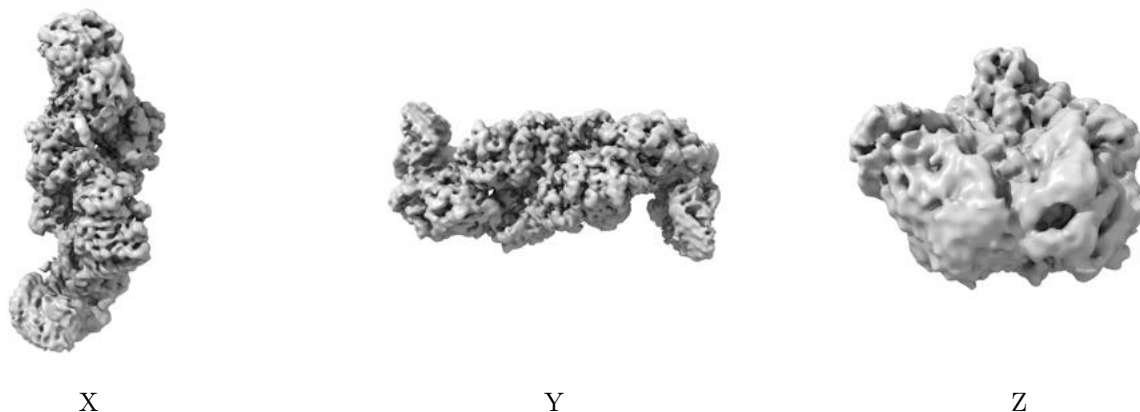
Z

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



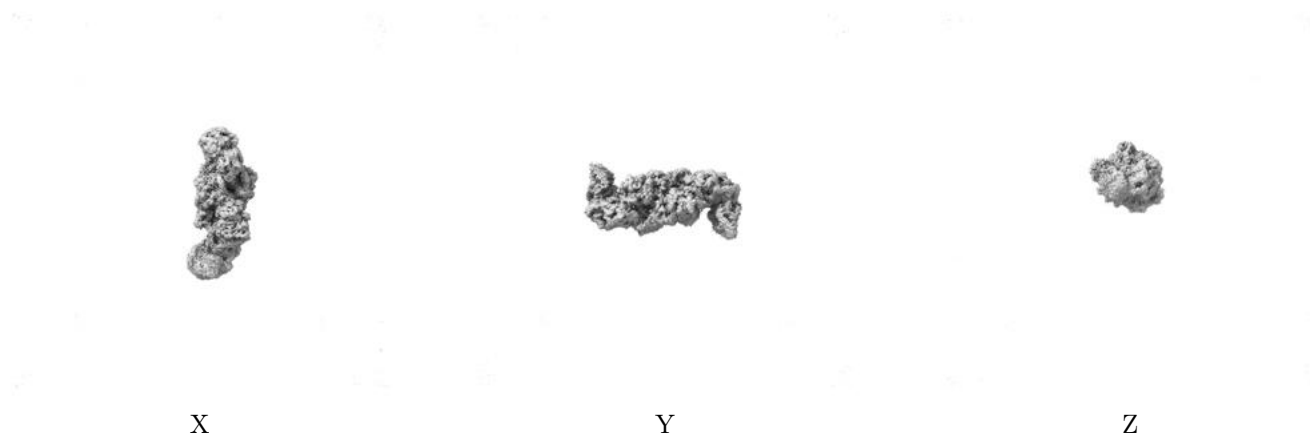
## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.265. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

### 6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

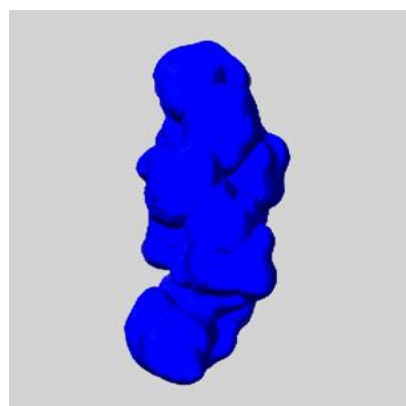
## 6.6 Mask visualisation [i](#)

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

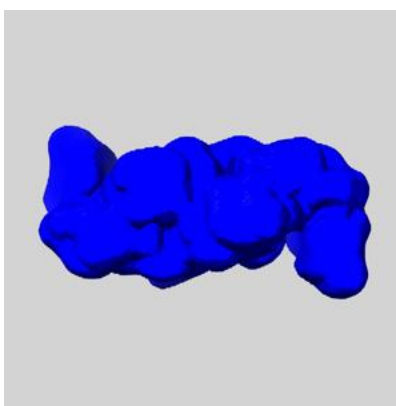
A mask typically either:

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

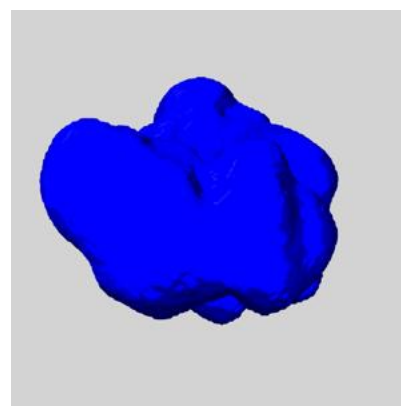
### 6.6.1 emd\_43356\_msk\_1.map [i](#)



X



Y



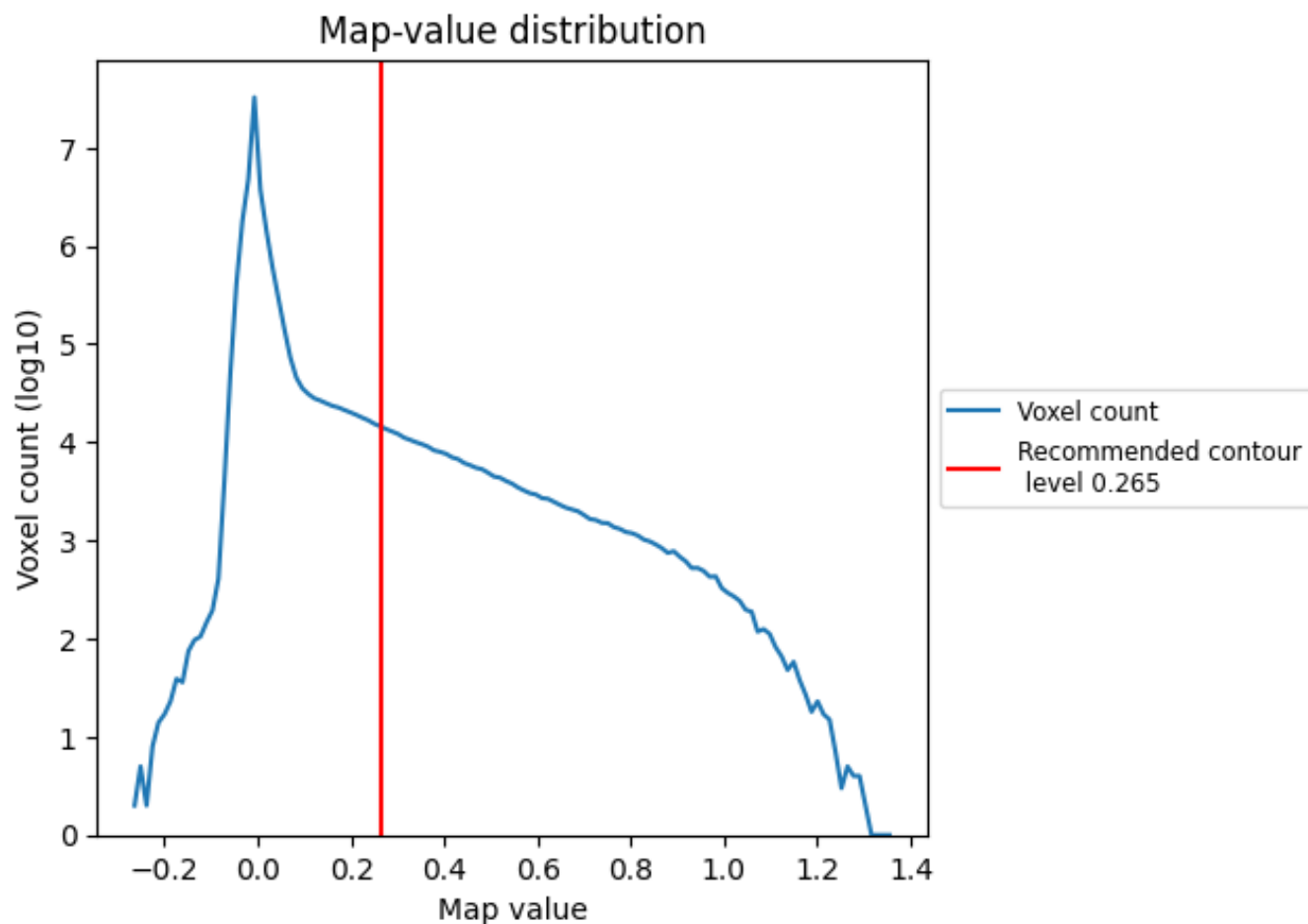
Z



## 7 Map analysis [i](#)

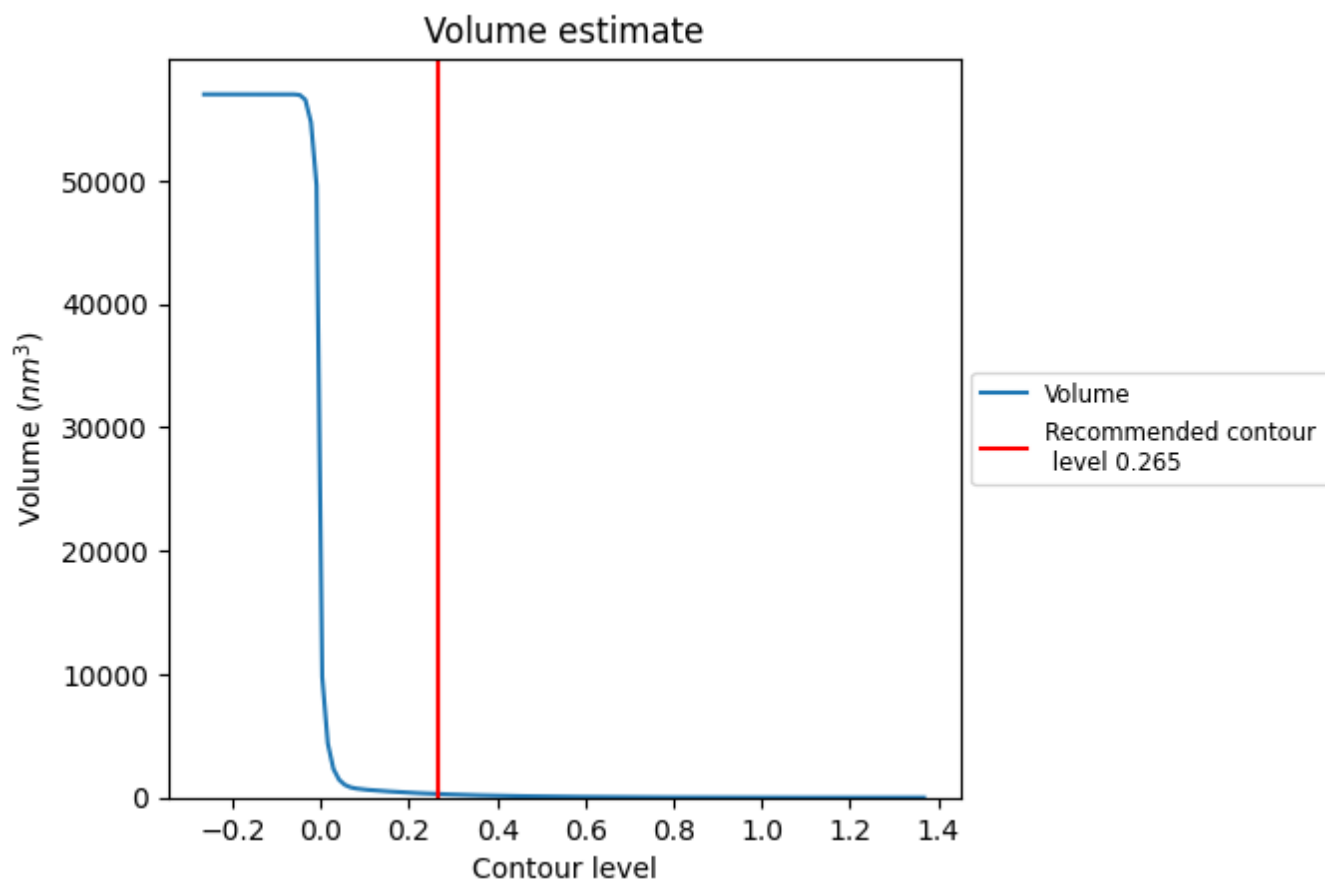
This section contains the results of statistical analysis of the map.

### 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.

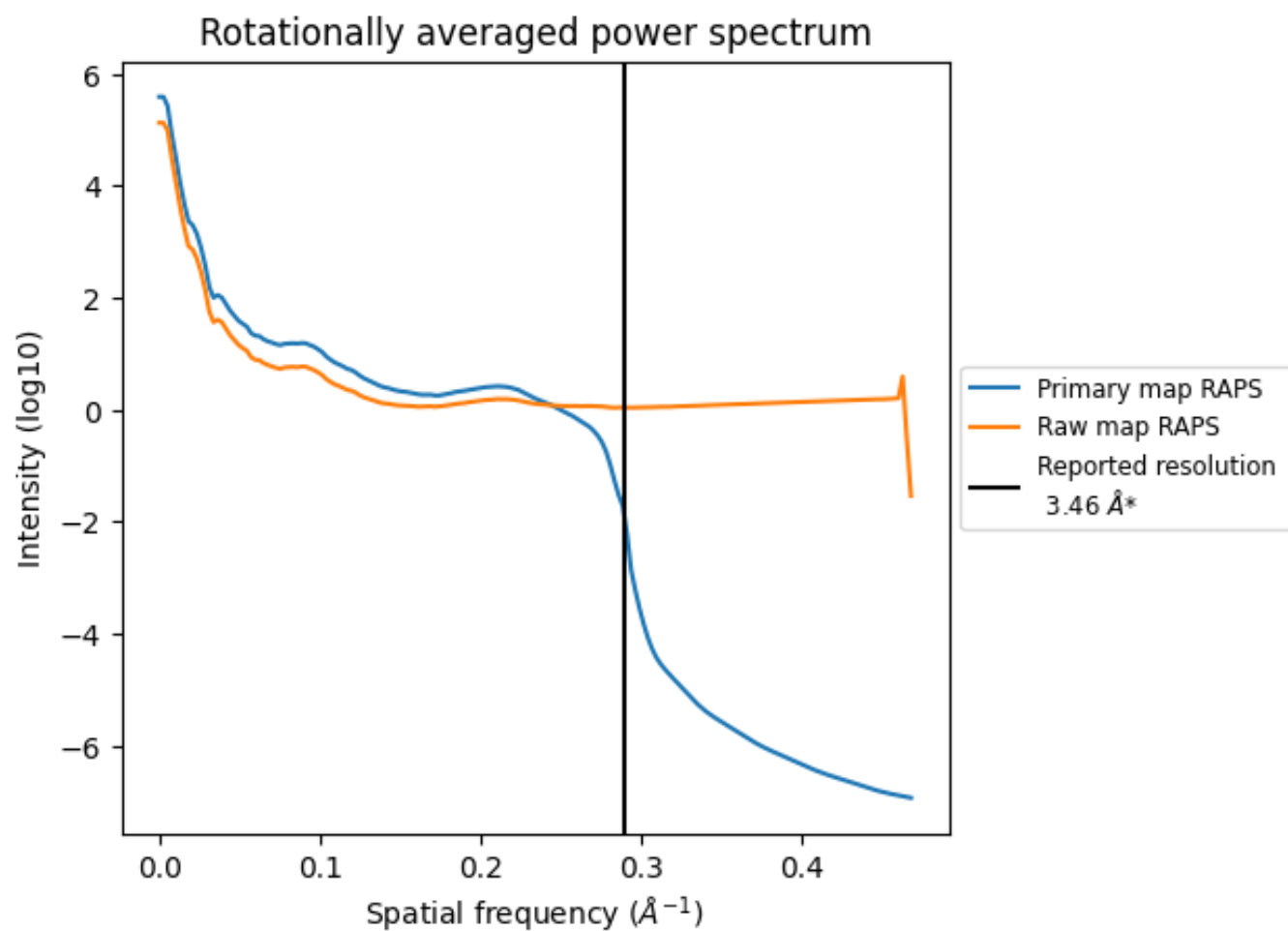
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 290  $\text{nm}^3$ ; this corresponds to an approximate mass of 262 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 ⓘ

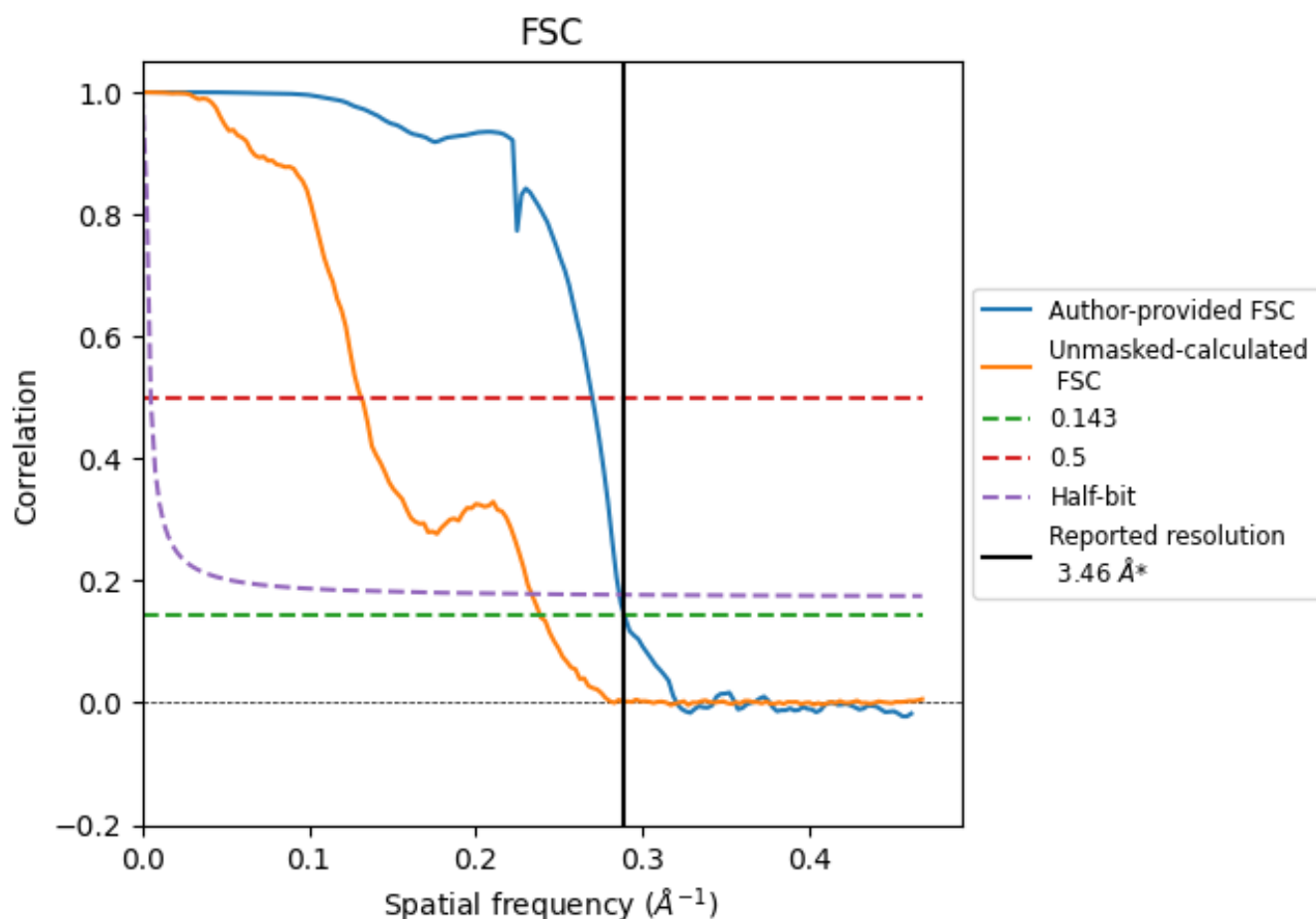


\*Reported resolution corresponds to spatial frequency of 0.289  $\text{\AA}^{-1}$

## 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 0.289  $\text{\AA}^{-1}$

## 8.2 Resolution estimates [i](#)

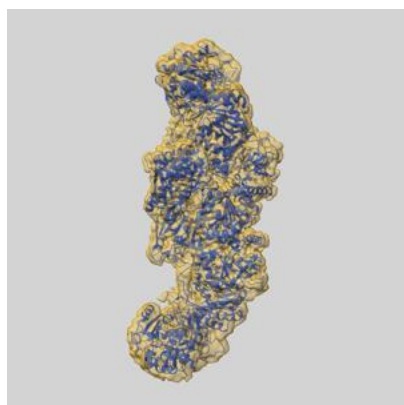
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.46	-	-
Author-provided FSC curve	3.46	3.71	3.49
Unmasked-calculated*	4.19	7.62	4.28

\*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 4.19 differs from the reported value 3.46 by more than 10 %

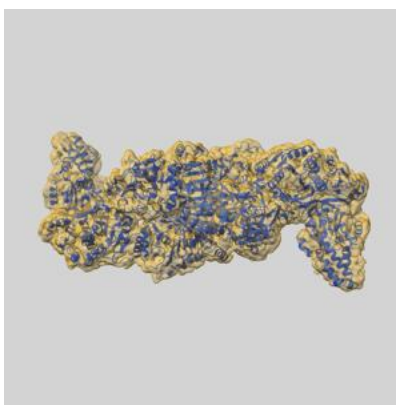
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43356 and PDB model 8VMD. Per-residue inclusion information can be found in [section 3](#) on [page 7](#).

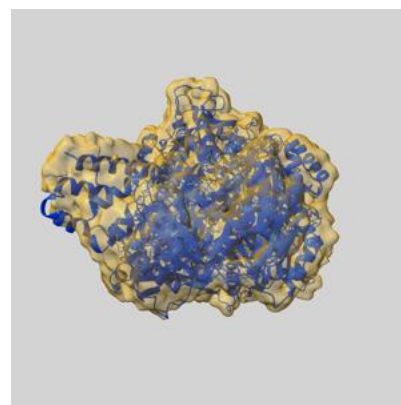
### 9.1 Map-model overlay [i](#)



X



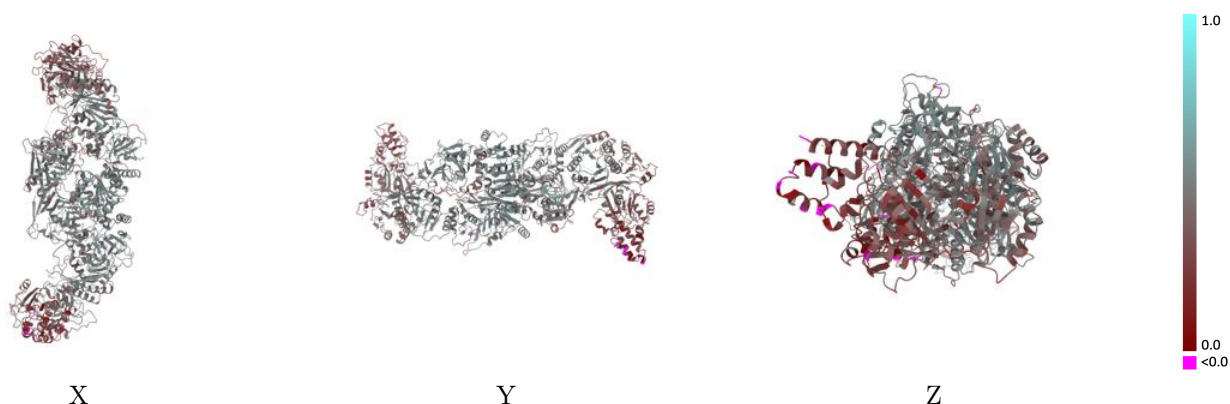
Y



Z

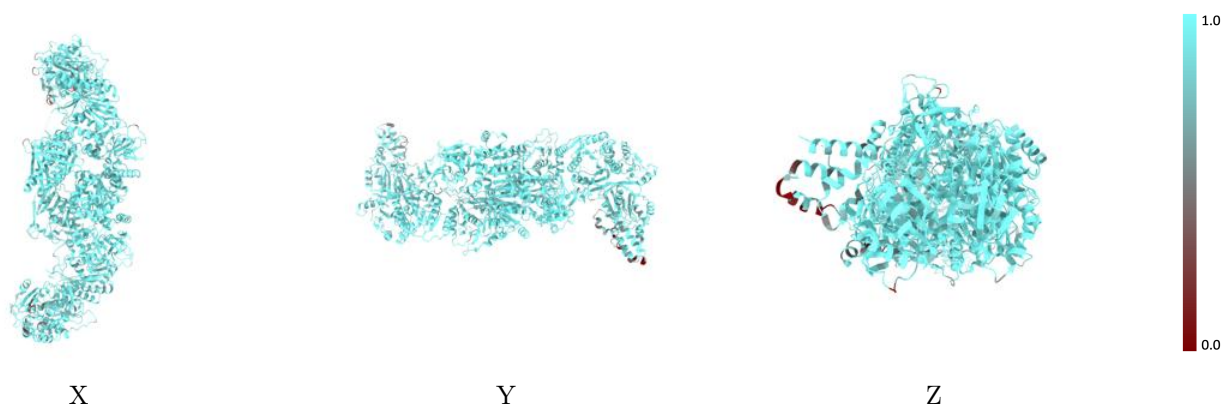
The images above show the 3D surface view of the map at the recommended contour level 0.265 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



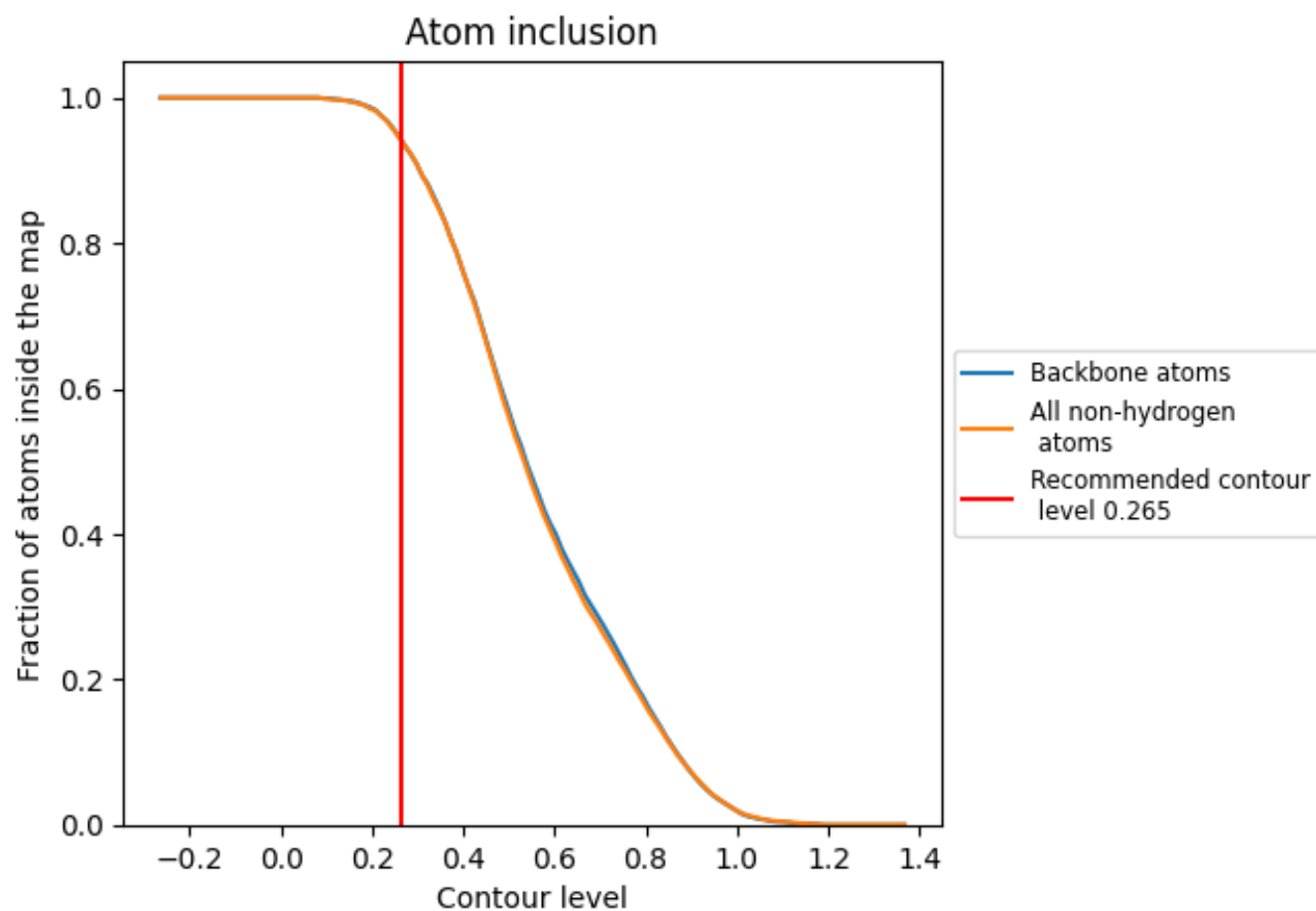
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.265).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 94% 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 (0.265) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9400	<div></div> 0.4210
A	<div></div> 0.9480	<div></div> 0.4310
B	<div></div> 0.9420	<div></div> 0.4110

