



wwPDB EM Validation Summary Report ⓘ

Jun 9, 2024 – 12:31 PM EDT

PDB ID : 8EYK
EMDB ID : EMD-28691
Title : Atomic model of the core modifying region of human fatty acid synthase in complex with TVB-2640
Authors : Hasan, S.M.N.; Keszei, A.; Mazhab-Jafari, M.T.
Deposited on : 2022-10-27
Resolution : 2.70 Å(reported)

This is a wwPDB EM Validation Summary Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

EMDB validation analysis	:	0.0.1.dev92
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

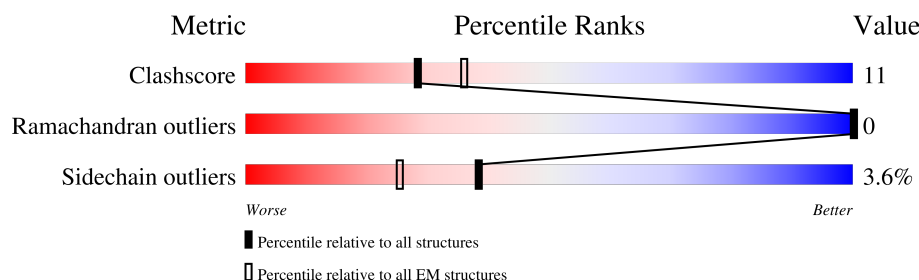
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 2.70 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	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	E	1670	
1	F	1670	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15386 atoms, of which 0 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.

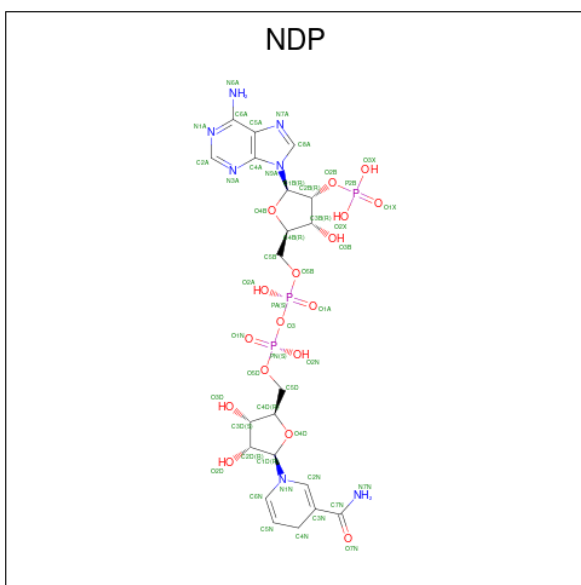
Mol	Chain	Residues	Atoms					AltConf	Trace
1	E	966	Total	C	N	O	S	0	0
			7179	4571	1268	1314	26		
1	F	1070	Total	C	N	O	S	0	0
			7949	5068	1398	1451	32		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	854	GLY	-	cloning artifact	UNP P49327
E	2512	LEU	-	cloning artifact	UNP P49327
E	2513	GLU	-	cloning artifact	UNP P49327
E	2514	SER	-	cloning artifact	UNP P49327
E	2515	ARG	-	cloning artifact	UNP P49327
E	2516	GLY	-	cloning artifact	UNP P49327
E	2517	PRO	-	cloning artifact	UNP P49327
E	2518	HIS	-	expression tag	UNP P49327
E	2519	HIS	-	expression tag	UNP P49327
E	2520	HIS	-	expression tag	UNP P49327
E	2521	HIS	-	expression tag	UNP P49327
E	2522	HIS	-	expression tag	UNP P49327
E	2523	HIS	-	expression tag	UNP P49327
F	854	GLY	-	cloning artifact	UNP P49327
F	2512	LEU	-	cloning artifact	UNP P49327
F	2513	GLU	-	cloning artifact	UNP P49327
F	2514	SER	-	cloning artifact	UNP P49327
F	2515	ARG	-	cloning artifact	UNP P49327
F	2516	GLY	-	cloning artifact	UNP P49327
F	2517	PRO	-	cloning artifact	UNP P49327
F	2518	HIS	-	expression tag	UNP P49327
F	2519	HIS	-	expression tag	UNP P49327
F	2520	HIS	-	expression tag	UNP P49327
F	2521	HIS	-	expression tag	UNP P49327
F	2522	HIS	-	expression tag	UNP P49327
F	2523	HIS	-	expression tag	UNP P49327

-
- The chemical structure of X50 is a complex molecule. It features a central benzene ring (C13-C18) substituted with a nitrile group (C19-C22) and a cyclohexane ring (C11-C16). The cyclohexane ring is further substituted with a pyrazole ring (N15-N16, C23-C26) and a cyclobutane ring (C27-C30). The pyrazole ring is substituted with a methyl group (C31) and a methyl group (C32). The cyclobutane ring is substituted with a methyl group (C33) and a methyl group (C34). The nitrile group is represented by a blue nitrogen atom (N1) and a carbon atom (C19) triple-bonded to a carbon atom (C22) which is also triple-bonded to a nitrogen atom (N2).

- Molecule 3 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

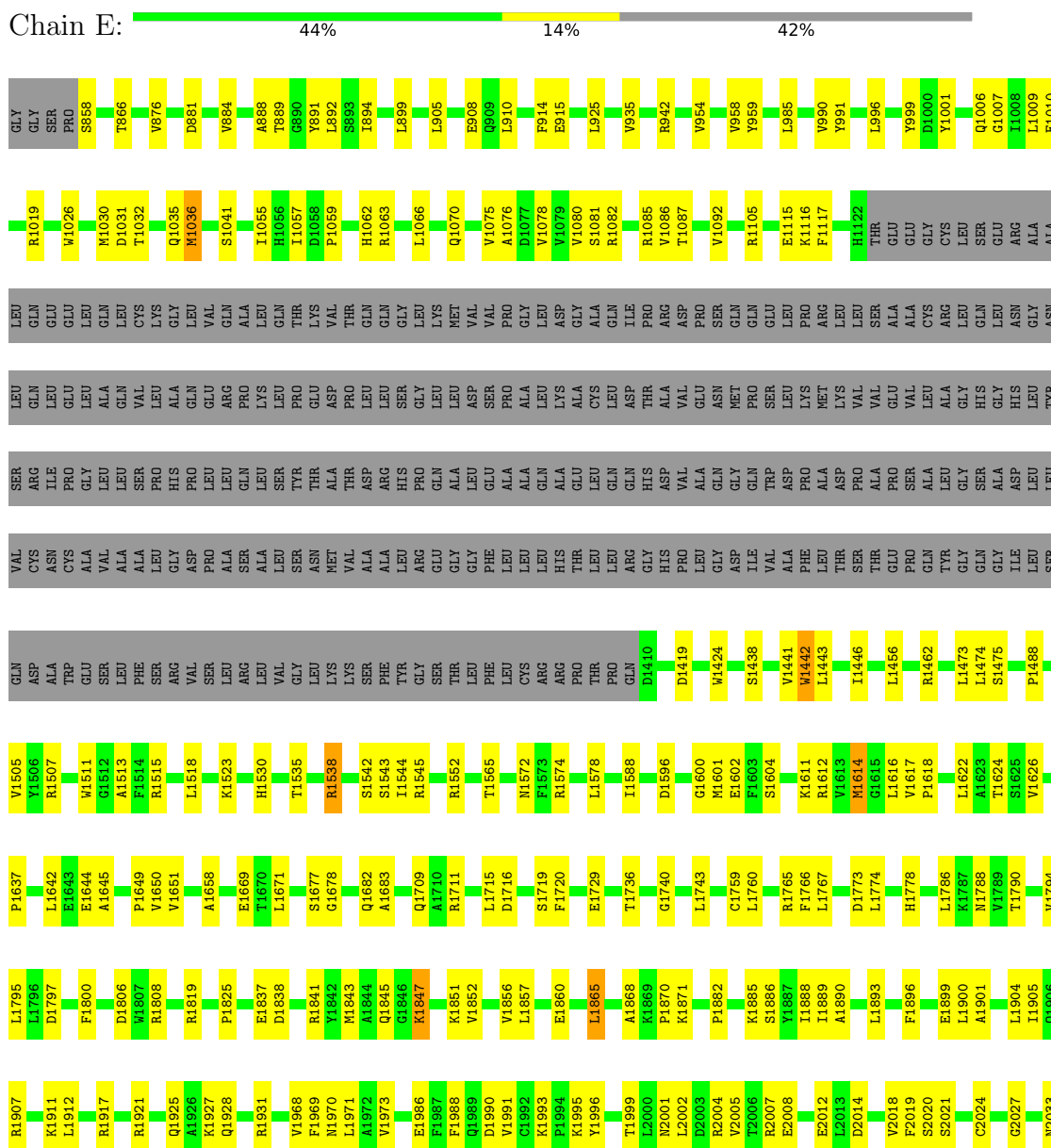


Mol	Chain	Residues	Atoms					AltConf
3	E	1	Total 48	C 21	N 7	O 17	P 3	0
3	E	1	Total 48	C 21	N 7	O 17	P 3	0
3	F	1	Total 48	C 21	N 7	O 17	P 3	0
3	F	1	Total 48	C 21	N 7	O 17	P 3	0

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





VAL	ARG	ALA	SER	PRO	ILE	LYS	ASP	P2054	R1921	L1796	T1697	L1563
SER	LEU	LEU	PRO	ALA	THR	GLU	SER	A2057	Q1925	E1802	T1698	V1566
ARG	LYS	PRO	ALA	THR	TYR	GLY	LEU	V2058	Q1925	SER	E1703	Y1567
GLY	THR	LEU	THR	THR	LEU	ALA	ASP	Q2059	R1930	SER	K1704	S1570
LEU	GLY	LYS	ASN	ASN	LEU	GLN	LEU			A1805		
ALA	GLY	GLY	ASN	GLN	GLN	GLN	GLY	A2062	V1937	V1811	Q1709	D1596
LEU	LEU	LEU	SER	CYS	THR	GLN	LEU	T2063	E1950	Q1815	A1710	Q1595
THR	GLY	THR	LEU	ARG	THR	THR	ASP	G2064	E1950	Q1815	R1711	
ARG	GLY	GLY	LEU	ALA	GLN	GLN	SER	D2065	A1960	R1819	L1715	D1716
GLY	VAL	VAL	PHE	ALA	LEU	LEU	MET	V2066	A1960	R1819	L1715	E1602
ASP	ALA	ASP	PRO	ALA	ASN	ASN	LEU		G1963	E1837	S1717	F1603
LEU	ALA	GLY	LEU	LEU	LEU	LEU	SER	L2069	G1963	E1837		
ALA	ASP	ASP	ASP	ASP	ASP	ARG	VAL	V2070	G1966	R1841	F1720	
ALA	PRO	PRO	PRO	ILE	ILE	LEU	VAL	E2071	G1966	R1841	A1721	R1606
THR	ASP	THR	THR	THR	THR	LEU	VAL			K1851	R1724	A1608
ASN	LEU	VAL	VAL	VAL	VAL	ASN	GLN	L2084	M1970	K1851	E1729	R1612
LEU	ILE	LEU	LEU	LEU	LEU	ASN	THR	P2085	L1971	V1856	E1729	V1613
SER	ILE	LEU	LEU	LEU	LEU	ASN	THR	Q2086	A1972	V1856	E1729	V1617
GLN	LYS	LEU	LEU	ALA	ALA	PRO	LEU	R2087	V1973	E1860	V1732	
VAL	VAL	THR	THR	ALA	ALA	GLY	GLY	W2088	D1977	P1861	V1732	
CYS	HIS	THR	THR	TYR	TYR	GLY	ARG		G1978	E1862	T1736	
ASP	GLN	GLN	GLN	TYR	TYR	THR	LEU	V2105		F1862	T1736	
GLY	GLY	GLY	SER	ILE	ASP	LEU	ASN	L2106	M1982	K1866		
LYS	LEU	LEU	TYR	ASP	CYS	LEU	LEU			GLY	V1741	T1624
VAL	ASP	ASP	ARG	ARG	ILE	MET	VAL	A2112	Q1989	ALA	D1742	S1625
VAL	ARG	ARG	ALA	ALA	ILE	VAL	VAL	GLU	D1990	LYS	L1743	V1626
VAL	GLN	GLN	LYS	LYS	ARG	LEU	LEU	LYS	V1991	PRO	L1743	L1627
HIS	GLY	GLY	LEU	GLN	GLN	ASN	SER	ALA	V1991	PRO	L1743	L1628
VAL	VAL	THR	THR	VAL	VAL	SER	VAL	ALA		K1871	M1746	
ILE	LEU	PRO	PRO	GLN	GLN	VAL	ARG	ALA	K1995			F1632
GLY	PHE	GLY	GLY	PRO	PRO	GLN	GLU	TYR	Y1996	P1882	A1755	L1633
GLY	ALA	CYS	CYS	GLY	GLY	SER	VAL	ARG		A1883	S1756	W1634
ASP	ALA	GLY	GLY	GLY	GLY	SER	VAL	ASP	T1999	H1884		
HIS	ARG	ALA	ALA	PRO	PRO	GLU	GLU	ARG		K1885	G1759	P1637
THR	ARG	SER	ALA	TYR	TYR	ARG	LEU	ASP	L2002	S1886	L1760	
LEU	THR	PHE	ALA	ARG	ARG	PRO	THR	SER	D2003			W1640
LEU	TYR	GLY	VAL	VAL	VAL	LEU	LEU	GLN	R2004	T1889	R1765	T1641
GLY	TYR	ALA	ALA	ALA	ALA	PHE	ARG	ARG	V2005	A1890	F1766	L1642
GLY	LEU	GLY	GLY	GLY	GLY	LEU	LYS	ASP	T2006	L1893	L1767	
SER	ARG	ILE	ILE	TYR	TYR	VAL	LEU	LEU	R2007		E1768	P1649
LEU	ALA	CYS	CYS	TYR	TYR	HIS	GLN	VAL	E2008	L1893	I1769	V1650
LEU	ALA	PHE	PHE	PRO	PRO	PRO	GLU	GLU		F1896	G1770	V1651
GLY	ALA	GLY	GLY	GLY	GLY	ILE	LEU	ALA	E2012	G1897	K1771	
GLY	GLY	ALA	ALA	ALA	ALA	ILE	SER	VAL		A1901	F1772	Y1657
GLY	GLY	VAL	VAL	VAL	VAL	GLY	SER	VAL	R2026		D1773	A1658
GLY	VAL	CYS	CYS	CYS	CYS	GLY	LYS	ALA		L1904	L1774	L1659
ILE	THR	GLN	GLN	GLN	GLN	THR	LYS	ILE	G2030	L1904	M1782	R1662
ILE	THR	PHE	PHE	PHE	PHE	THR	ASP	LEU	Q2031	I1905	A1783	G1663
ILE	THR	GLU	GLU	GLU	GLU	VAL	GLY	GLY	S2032	Q1906	I1784	R1664
ILE	THR	GLU	GLU	GLU	GLU	VAL	ALA	ILE	N2033	V1909	K1787	V1666
HIS	LYS	ASP	ASP	ASP	ASP	HIS	SER	ASP	N2038	Q1910		
THR	LYS	THR	THR	THR	THR	SER	GLY	GLY	S2039	K1911	T1790	E1669
THR	LYS	THR	THR	THR	THR	LEU	LEU	LEU				T1670
LEU	GLY	GLY	GLY	GLY	GLY	ALA	ALA	ALA	E2042	T1915	G1793	L1671
ALA	ASN	ASN	ASN	ASN	ASN	CYS	CYS	ALA	R2043	S1916	V1794	
VAL	VAL	VAL	VAL	VAL	VAL	PRO	PRO	VAL		R1917		
PRO	PRO	PRO	PRO	PRO	PRO	THR	THR	THR	R2048	S1918	L1795	H1674
ARG	ARG	ARG	ARG	ARG	ARG	PRO	PRO	PRO				

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	311983	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50.76	Depositor
Minimum defocus (nm)	600	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	6.168	Depositor
Minimum map value	-3.725	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.176	Depositor
Recommended contour level	0.341	Depositor
Map size (\AA)	257.5, 257.5, 257.5	wwPDB
Map dimensions	250, 250, 250	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.03, 1.03, 1.03	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, X5O

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	E	0.29	0/7344	0.50	0/10015
1	F	0.29	0/8119	0.51	2/11061 (0.0%)
All	All	0.29	0/15463	0.50	2/21076 (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	F	1071	ASP	CB-CG-OD1	6.05	123.74	118.30
1	F	1497	LEU	CA-CB-CG	5.23	127.34	115.30

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	E	7179	0	6896	149	0
1	F	7949	0	7691	173	0
2	E	33	0	0	0	0
2	F	33	0	0	1	0
3	E	96	0	47	7	0
3	F	96	0	50	10	0
All	All	15386	0	14684	317	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 11.

The worst 5 of 317 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:F:1915:THR:HG22	3:F:2603:NDP:H2A	1.49	0.93
1:E:1991:VAL:HG11	1:E:2033:ASN:HB2	1.55	0.89
1:F:1991:VAL:HG11	1:F:2033:ASN:HB2	1.65	0.78
1:F:1716:ASP:OD1	1:F:1717:SER:N	2.18	0.77
1:F:1233:GLU:O	1:F:1461:ARG:NH1	2.18	0.77

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	E	960/1670 (58%)	942 (98%)	18 (2%)	0	100	100
1	F	1052/1670 (63%)	1027 (98%)	25 (2%)	0	100	100
All	All	2012/3340 (60%)	1969 (98%)	43 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	719/1392 (52%)	700 (97%)	19 (3%)	46	75
1	F	801/1392 (58%)	766 (96%)	35 (4%)	28	56
All	All	1520/2784 (55%)	1466 (96%)	54 (4%)	38	64

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	1444	LYS
1	F	1606	ARG
1	F	2008	GLU
1	F	1462	ARG
1	F	1563	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	E	1530	HIS
1	E	1555	GLN
1	F	1476	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	X5O	F	2601	-	36,37,37	1.94	8 (22%)	48,53,53	2.91	9 (18%)
2	X5O	E	2601	-	36,37,37	1.97	9 (25%)	48,53,53	2.94	8 (16%)
3	NDP	F	2603	-	45,52,52	3.90	21 (46%)	53,80,80	1.81	11 (20%)
3	NDP	E	2603	-	45,52,52	3.80	21 (46%)	53,80,80	1.76	10 (18%)
3	NDP	E	2602	-	45,52,52	3.81	18 (40%)	53,80,80	1.57	9 (16%)
3	NDP	F	2602	-	45,52,52	3.79	17 (37%)	53,80,80	1.81	11 (20%)

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	X5O	F	2601	-	-	3/22/38/38	1/5/5/5
2	X5O	E	2601	-	-	4/22/38/38	1/5/5/5
3	NDP	F	2603	-	-	11/30/77/77	0/5/5/5
3	NDP	E	2603	-	-	8/30/77/77	0/5/5/5
3	NDP	E	2602	-	-	12/30/77/77	0/5/5/5
3	NDP	F	2602	-	-	12/30/77/77	0/5/5/5

The worst 5 of 94 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2602	NDP	O4B-C1B	13.46	1.59	1.41
3	F	2603	NDP	O4B-C1B	13.17	1.59	1.41
3	F	2602	NDP	O4B-C1B	12.76	1.58	1.41
3	E	2603	NDP	O4B-C1B	11.86	1.57	1.41
3	F	2602	NDP	C2D-C3D	-10.80	1.23	1.53

The worst 5 of 58 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2601	X5O	C12-C13-C16	-13.49	81.17	112.79
2	F	2601	X5O	C12-C13-C16	-12.73	82.95	112.79
2	F	2601	X5O	C14-C13-C16	9.47	135.00	112.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2601	X5O	C14-C13-C16	8.94	133.76	112.79
2	F	2601	X5O	C27-N26-N25	7.16	108.80	105.31

There are no chirality outliers.

5 of 50 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	2601	X5O	C06-C05-C24-N25
2	E	2601	X5O	C06-C05-C24-N28
2	F	2601	X5O	C06-C05-C24-N28
3	E	2602	NDP	C5B-O5B-PA-O2A
3	E	2602	NDP	C5B-O5B-PA-O3

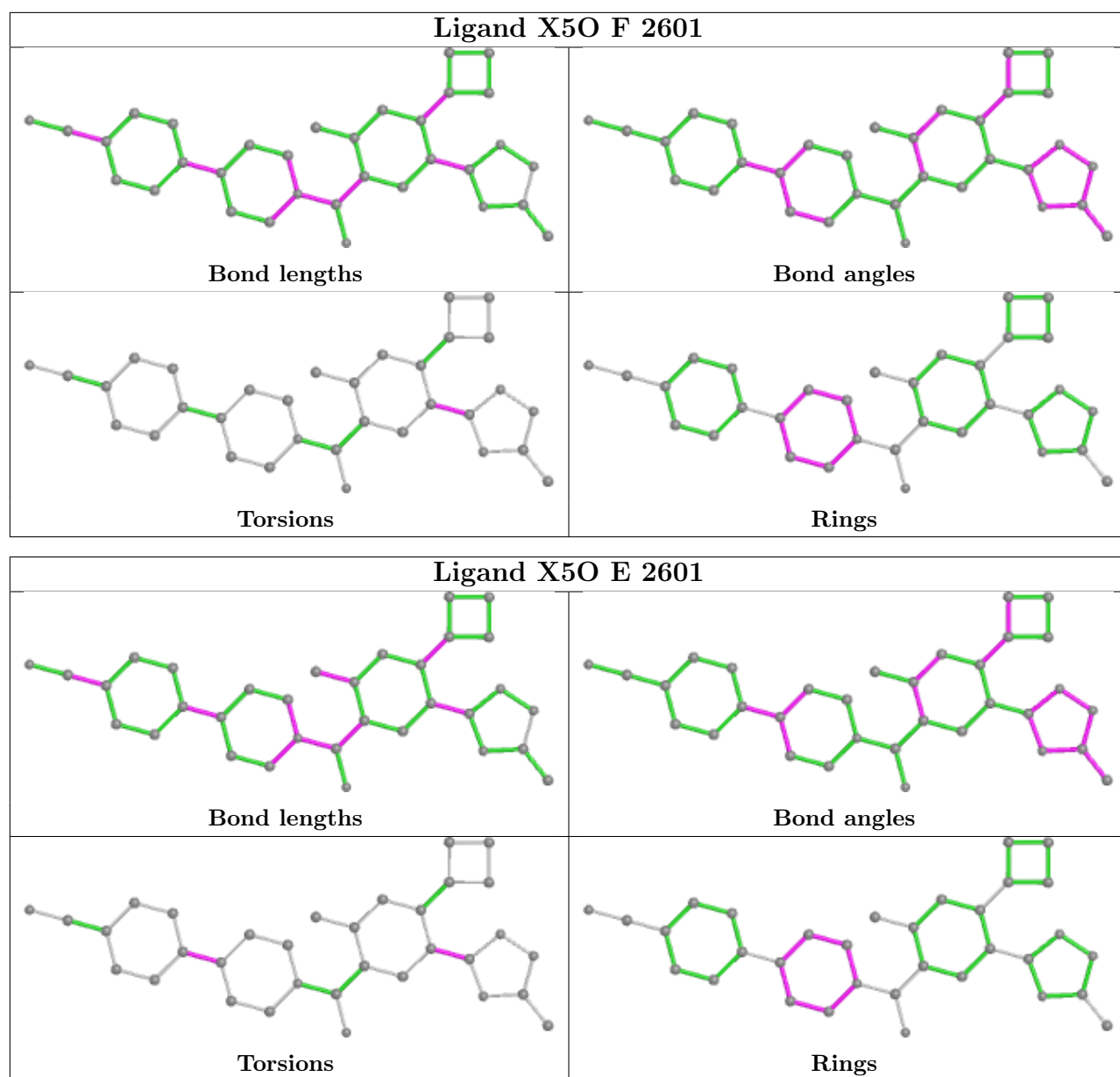
All (2) ring outliers are listed below:

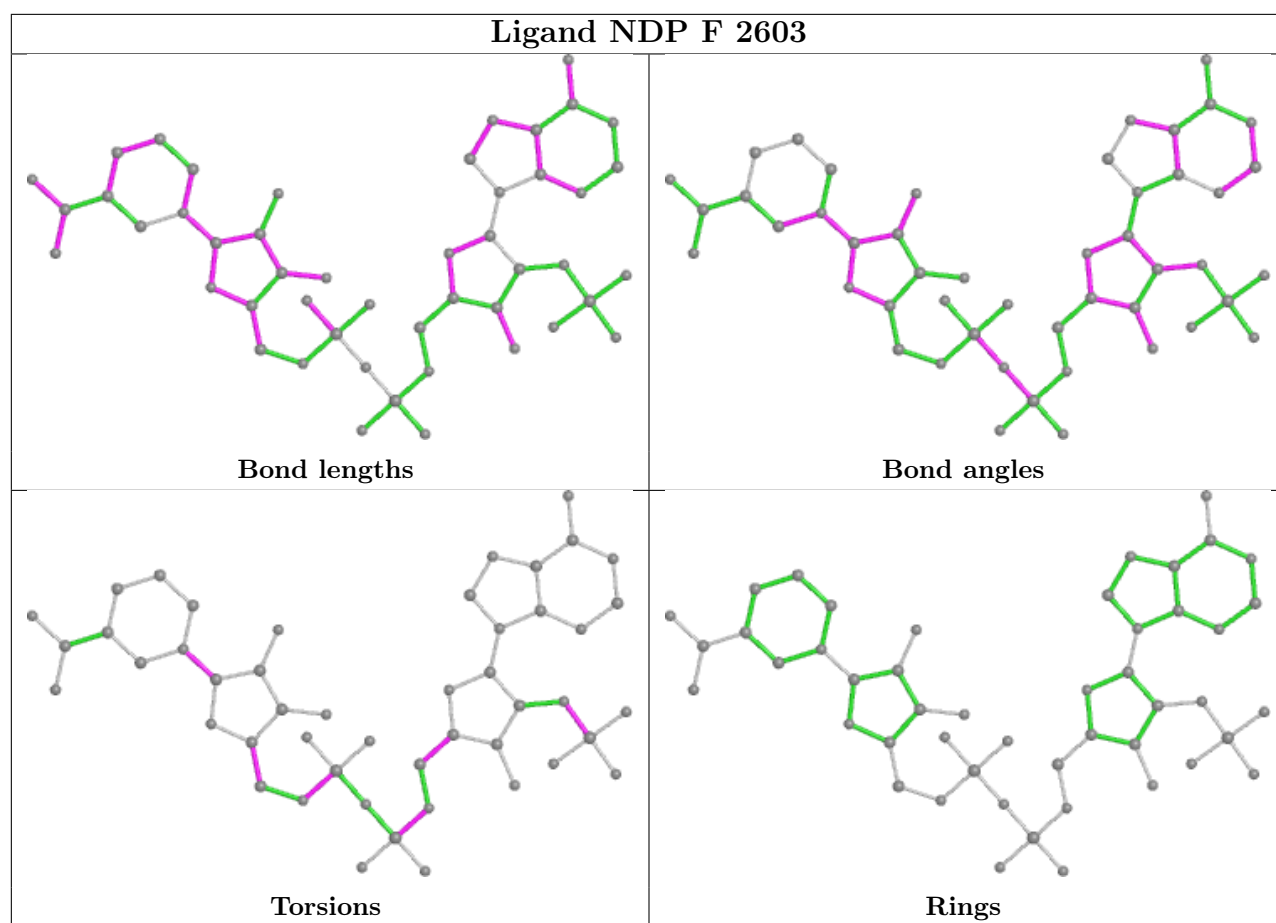
Mol	Chain	Res	Type	Atoms
2	E	2601	X5O	C11-C12-C13-C14-C15-N10
2	F	2601	X5O	C11-C12-C13-C14-C15-N10

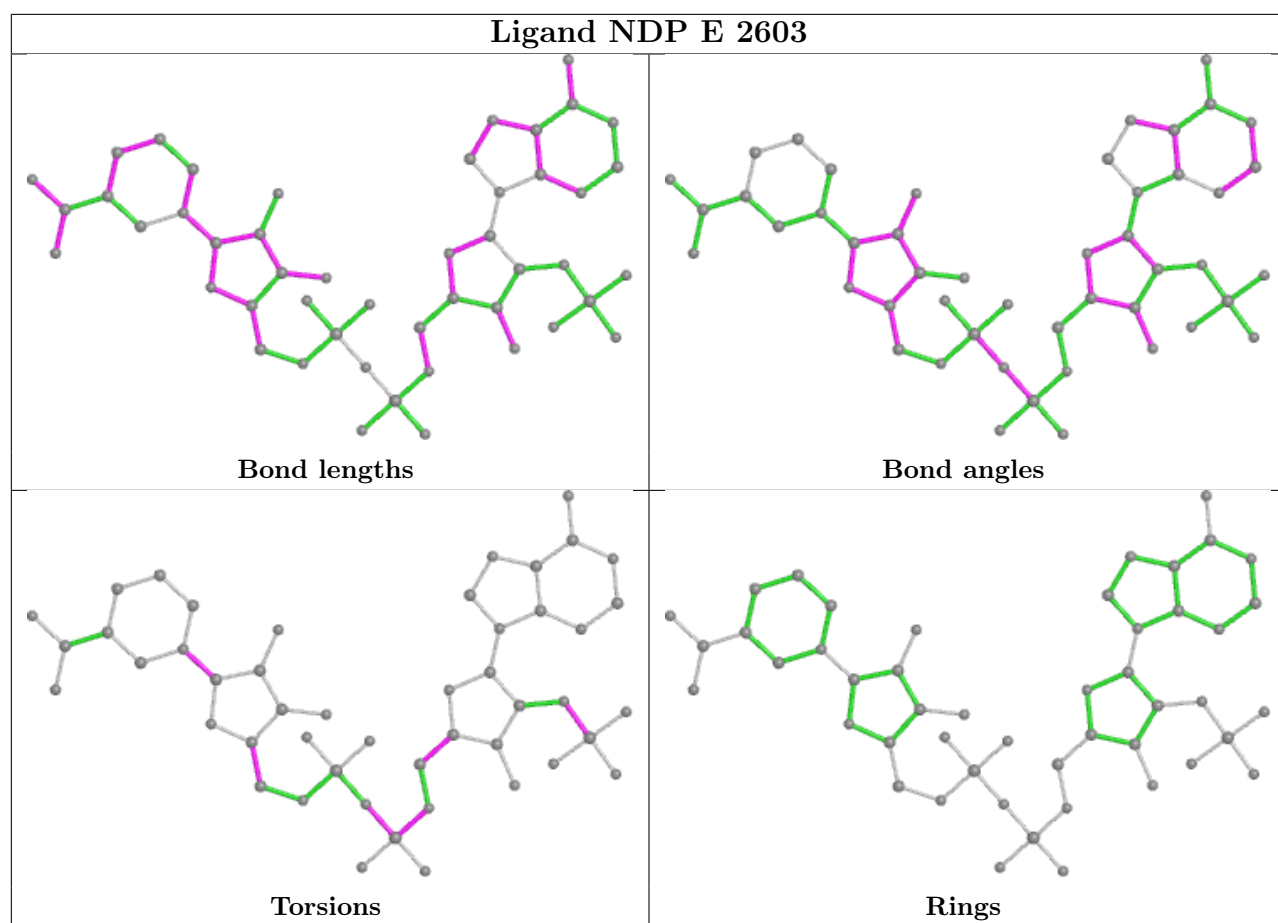
5 monomers are involved in 18 short contacts:

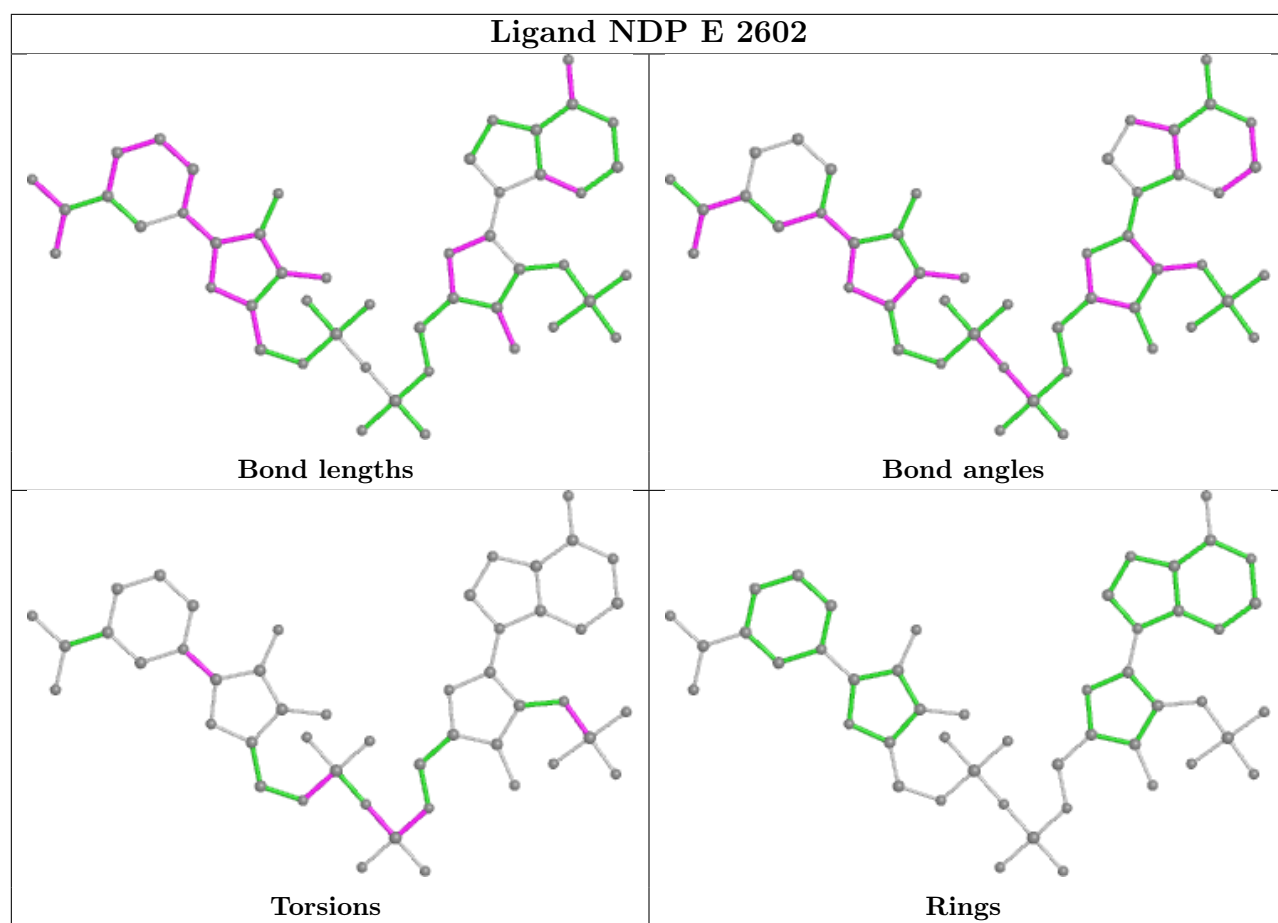
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	2601	X5O	1	0
3	F	2603	NDP	5	0
3	E	2603	NDP	6	0
3	E	2602	NDP	1	0
3	F	2602	NDP	5	0

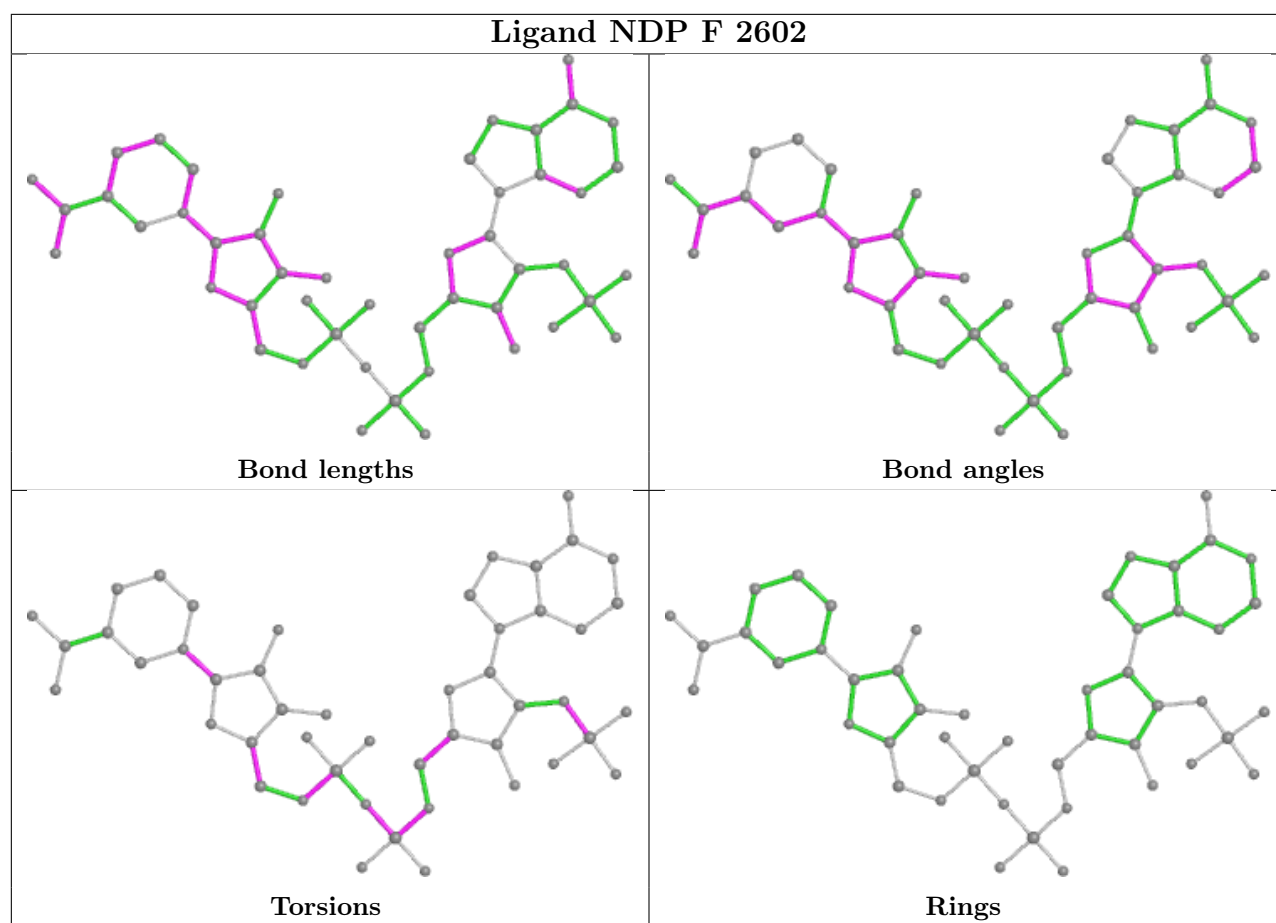
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

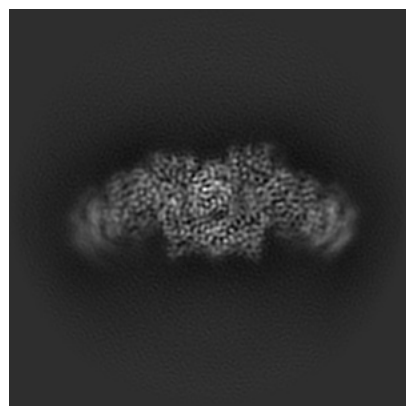
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28691. These allow visual inspection of the internal detail of the map and identification of artifacts.

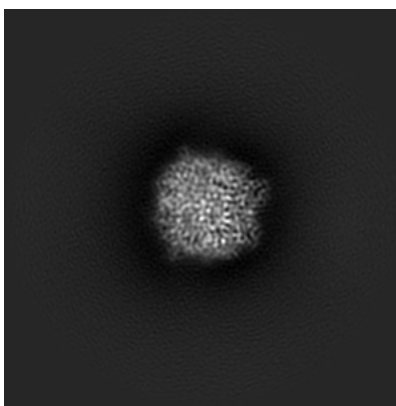
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

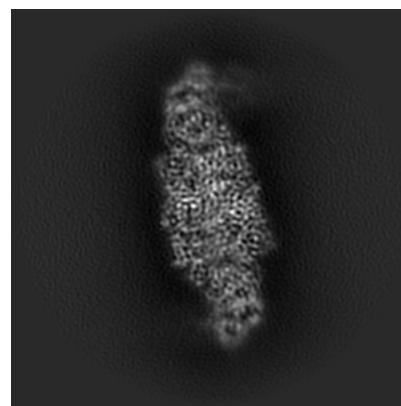
6.1.1 Primary map



X

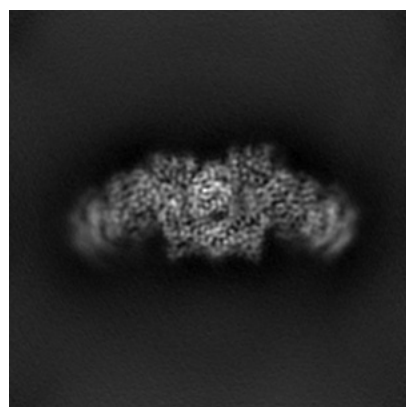


Y

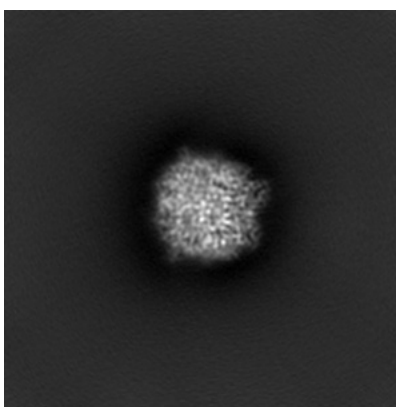


Z

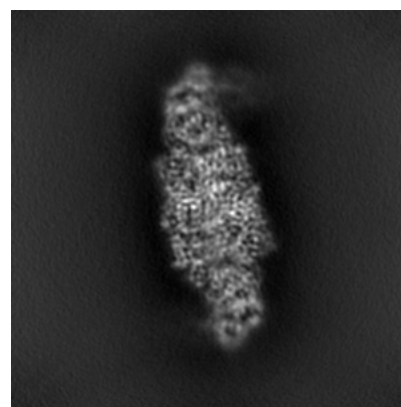
6.1.2 Raw map



X



Y

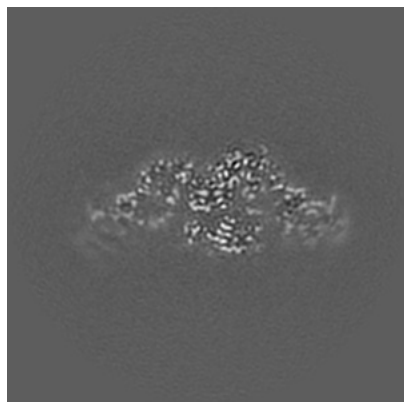


Z

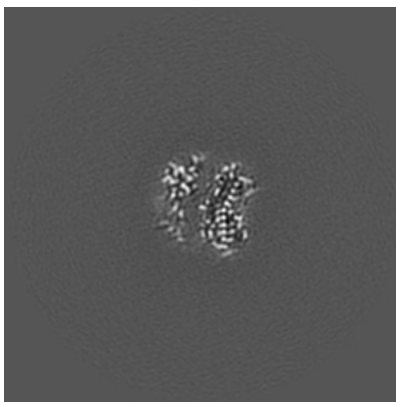
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

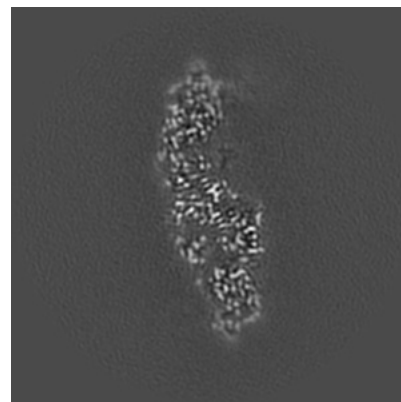
6.2.1 Primary map



X Index: 125

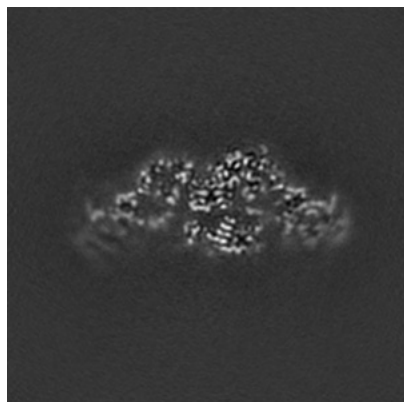


Y Index: 125

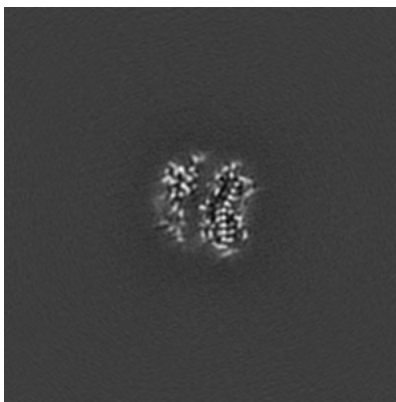


Z Index: 125

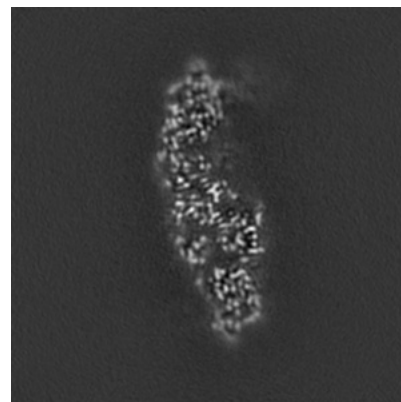
6.2.2 Raw map



X Index: 125



Y Index: 125

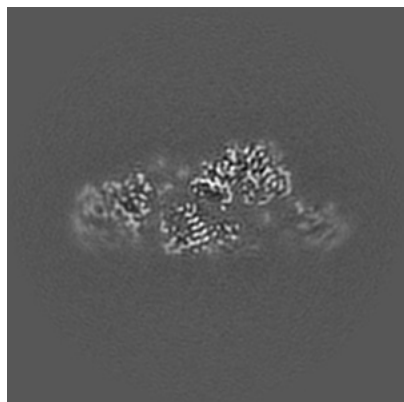


Z Index: 125

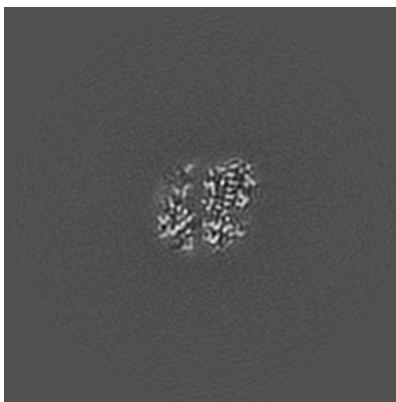
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

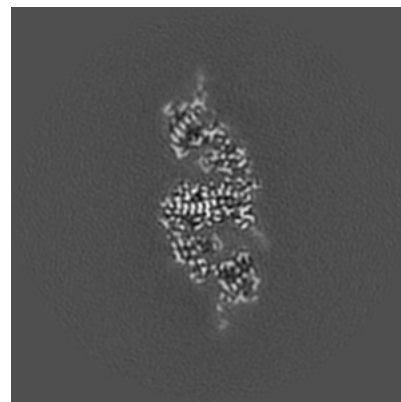
6.3.1 Primary map



X Index: 131

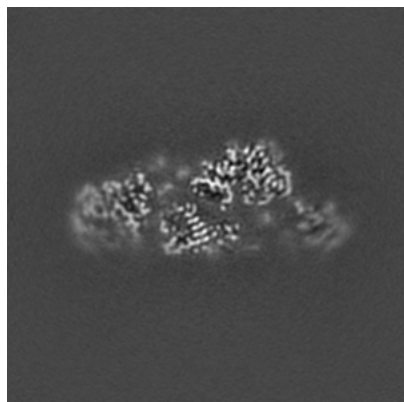


Y Index: 131

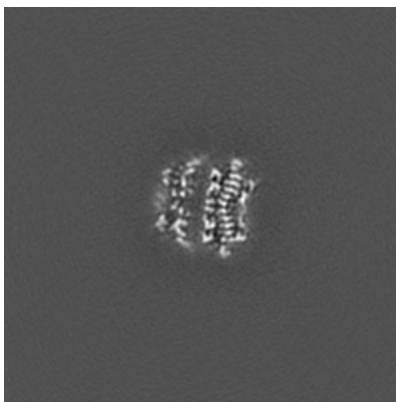


Z Index: 137

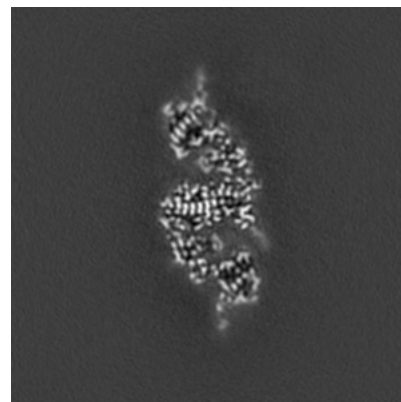
6.3.2 Raw map



X Index: 131



Y Index: 127

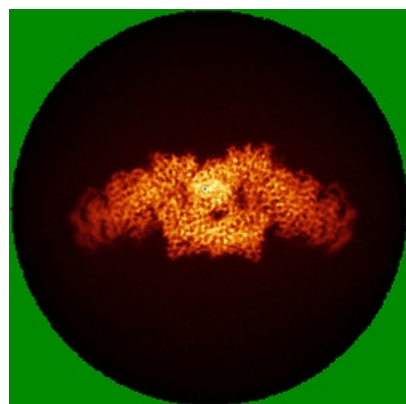


Z Index: 137

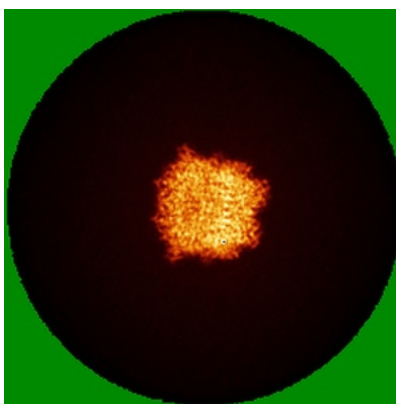
The images above show the largest variance slices of the map in three orthogonal directions.

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

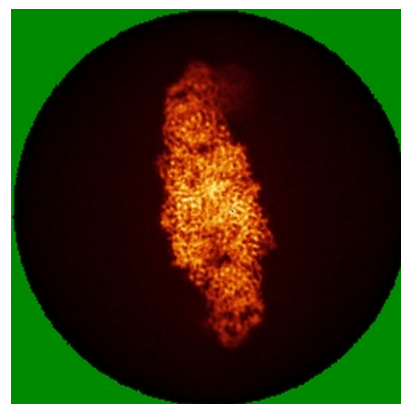
6.4.1 Primary map



X

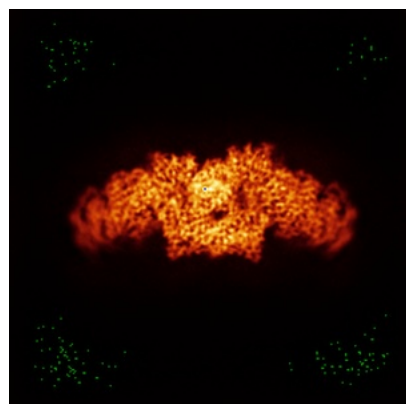


Y

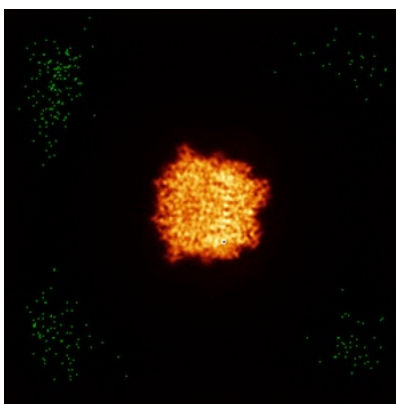


Z

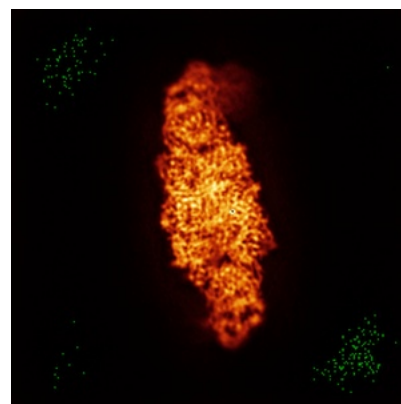
6.4.2 Raw map



X



Y

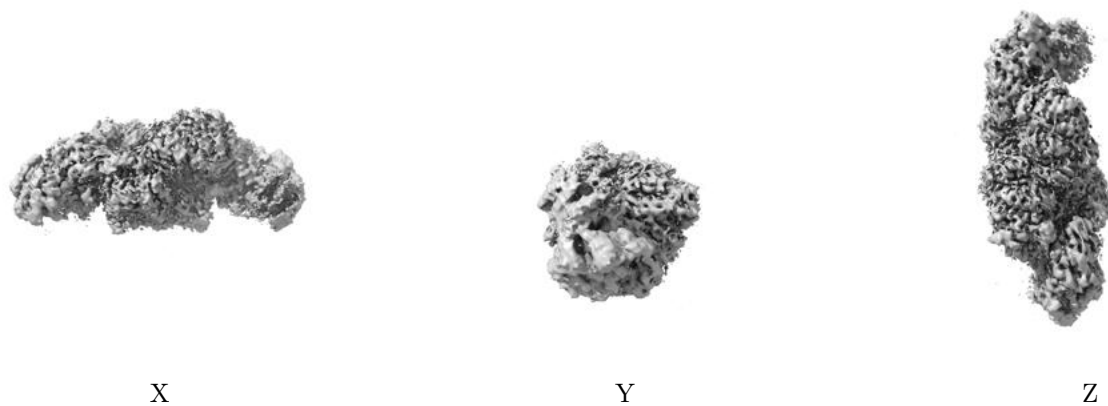


Z

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.

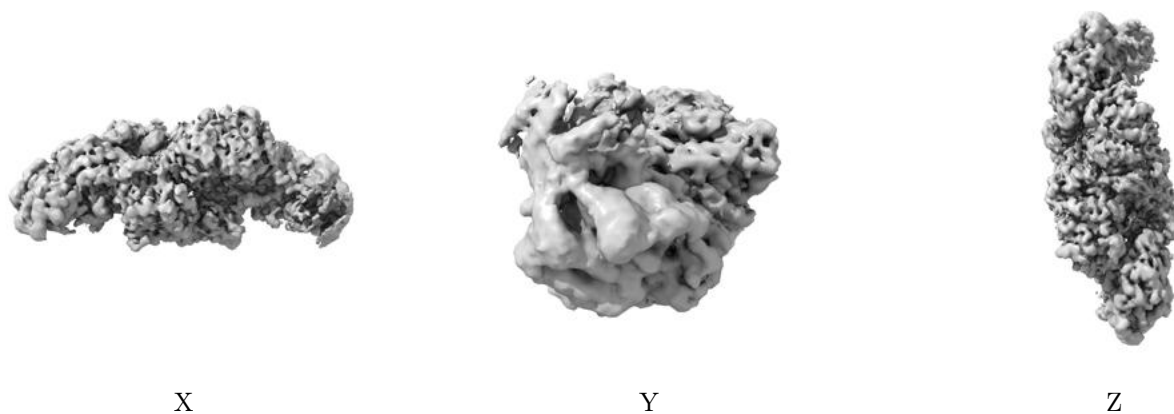
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.341. 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.

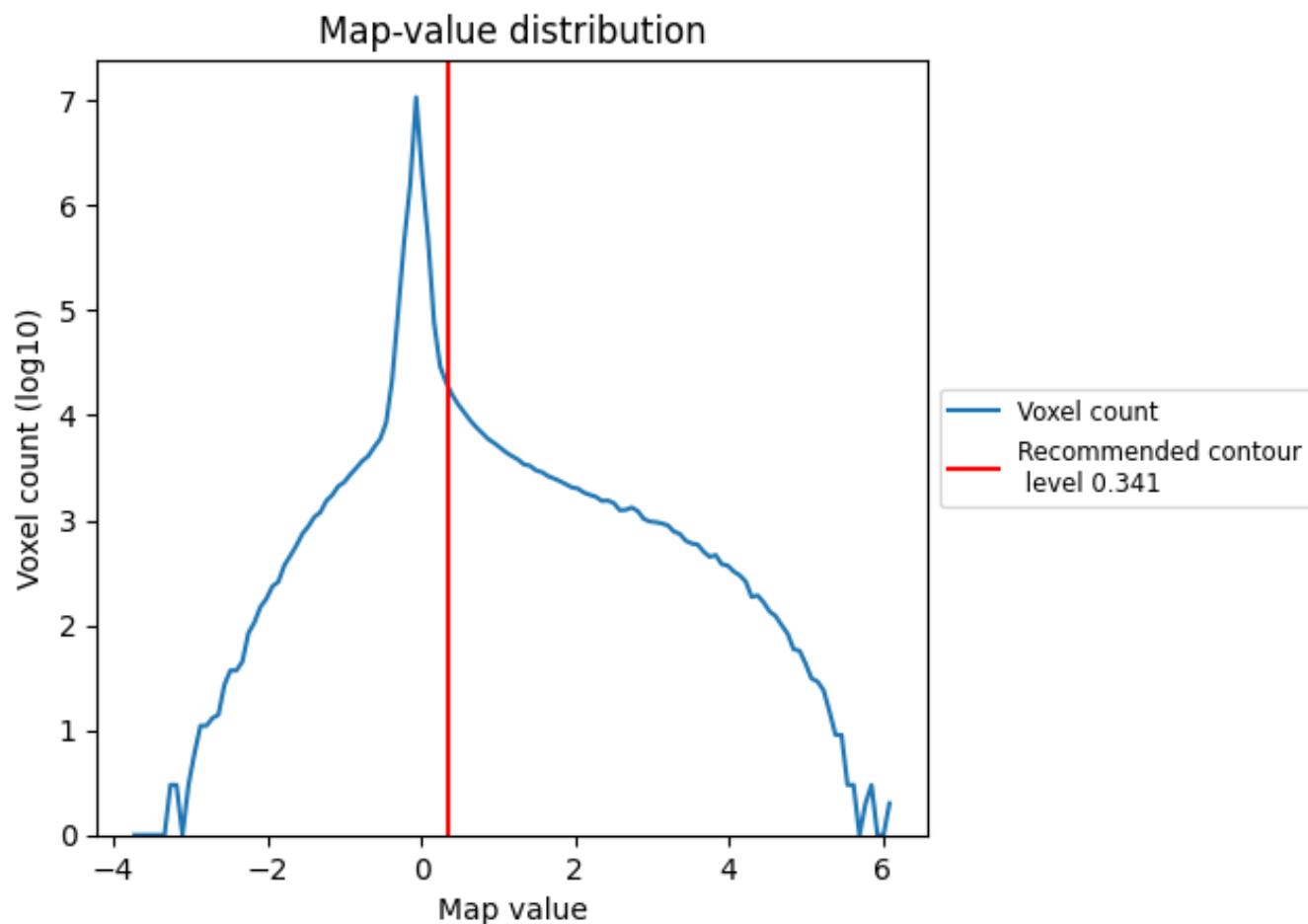
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

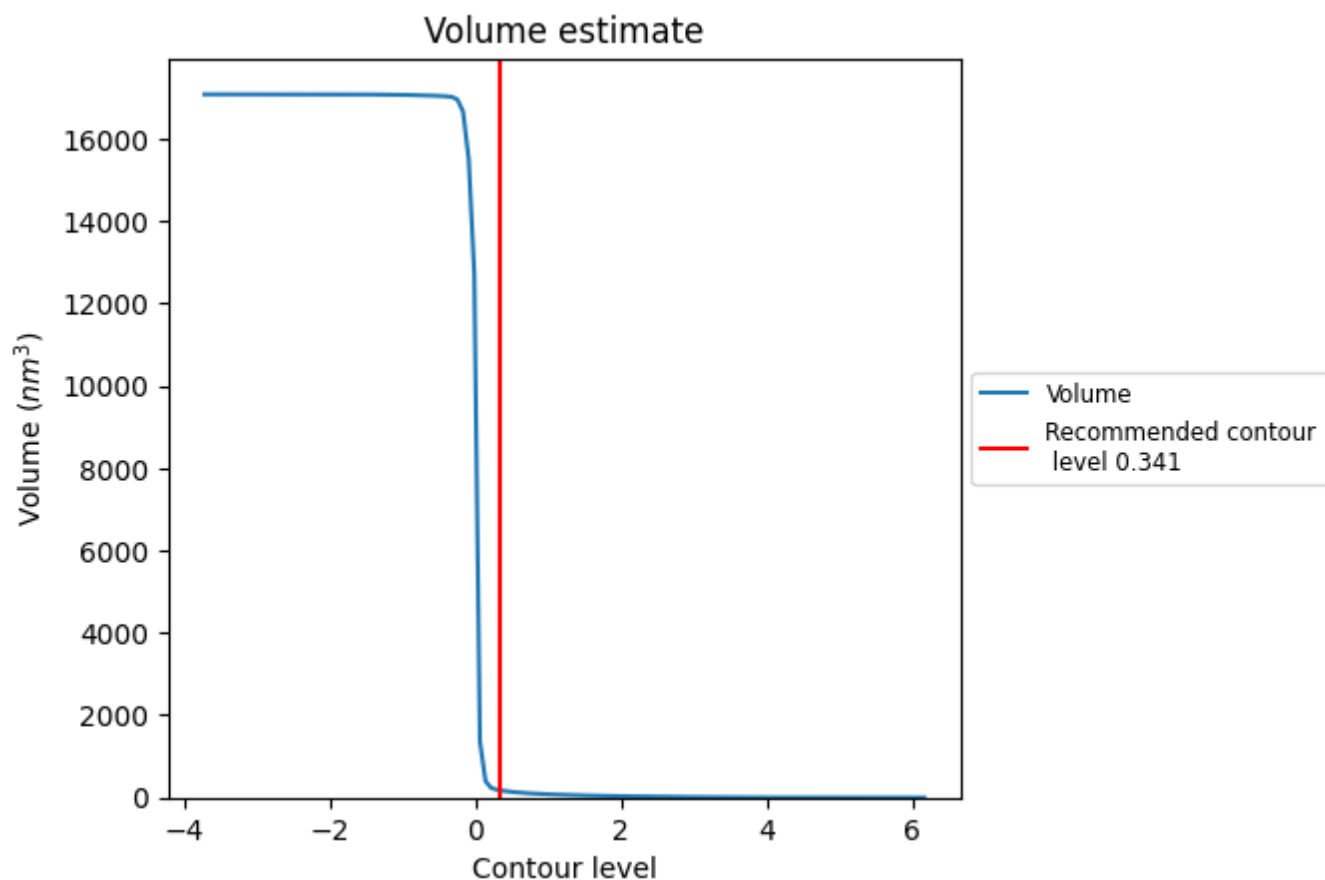
This section contains the results of statistical analysis of the map.

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.

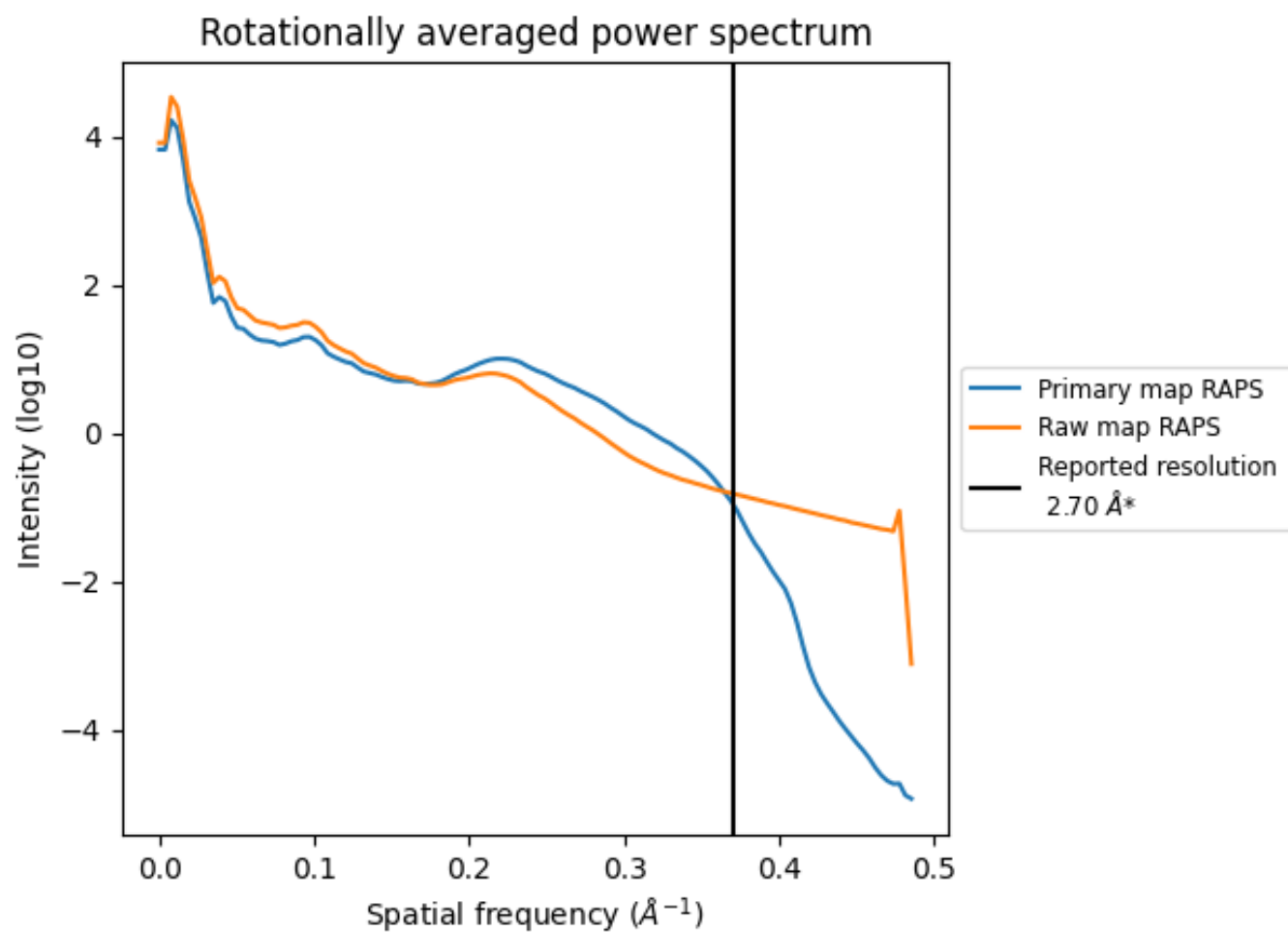
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 177 nm³; this corresponds to an approximate mass of 160 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 ⓘ

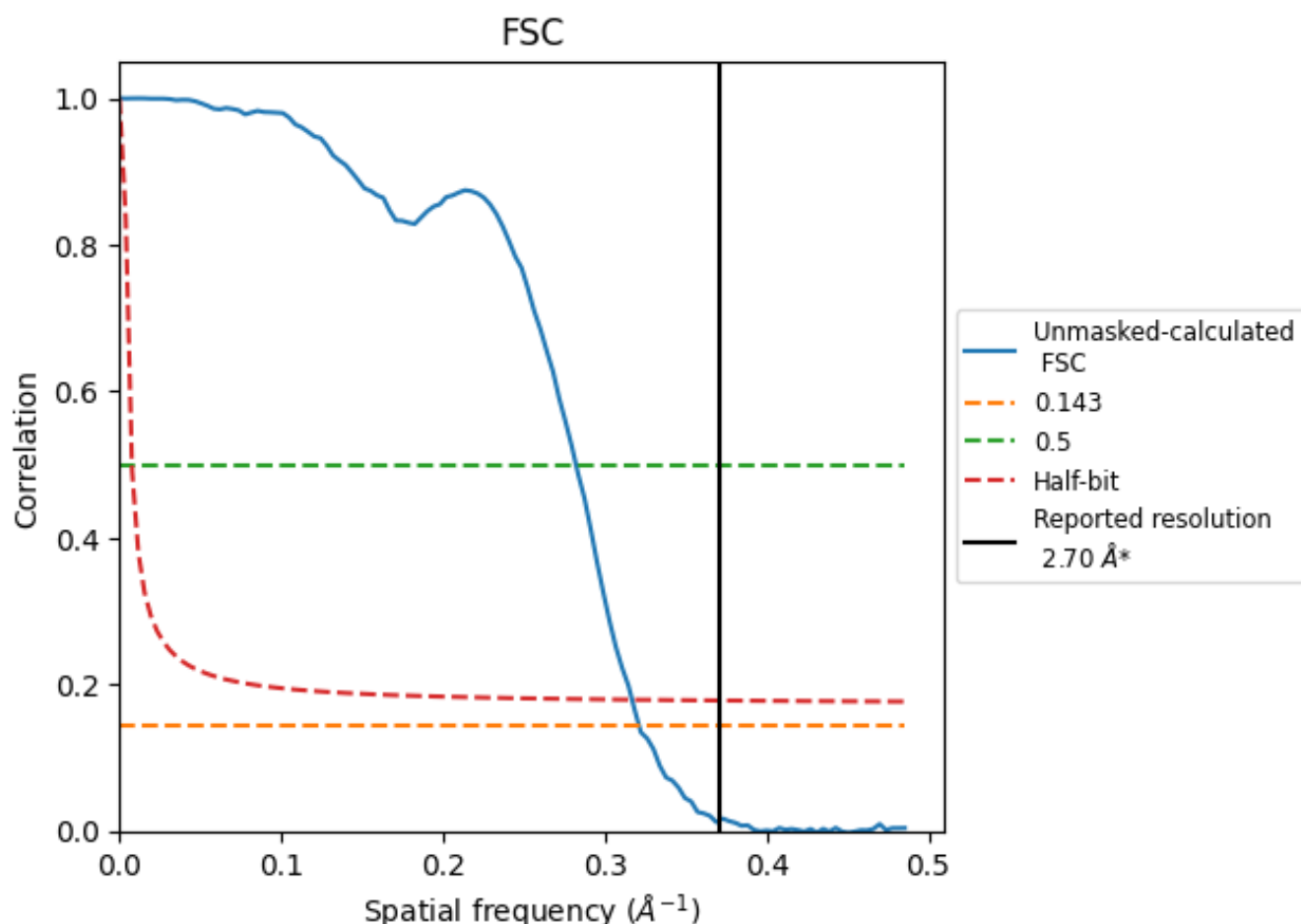


*Reported resolution corresponds to spatial frequency of 0.370 Å⁻¹

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 0.370 \AA^{-1}

8.2 Resolution estimates [i](#)

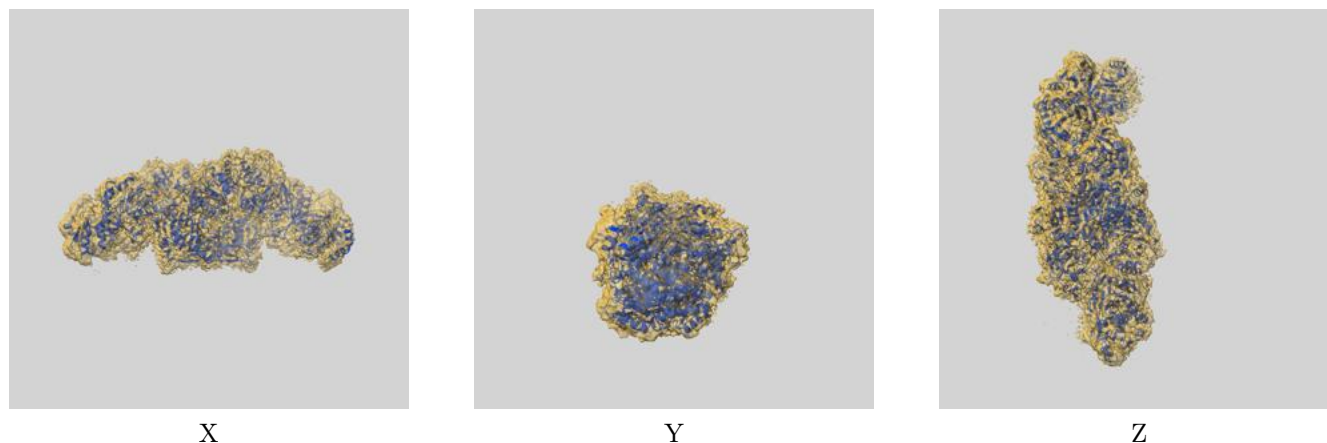
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.11	3.54	3.16

*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 3.11 differs from the reported value 2.7 by more than 10 %

9 Map-model fit [i](#)

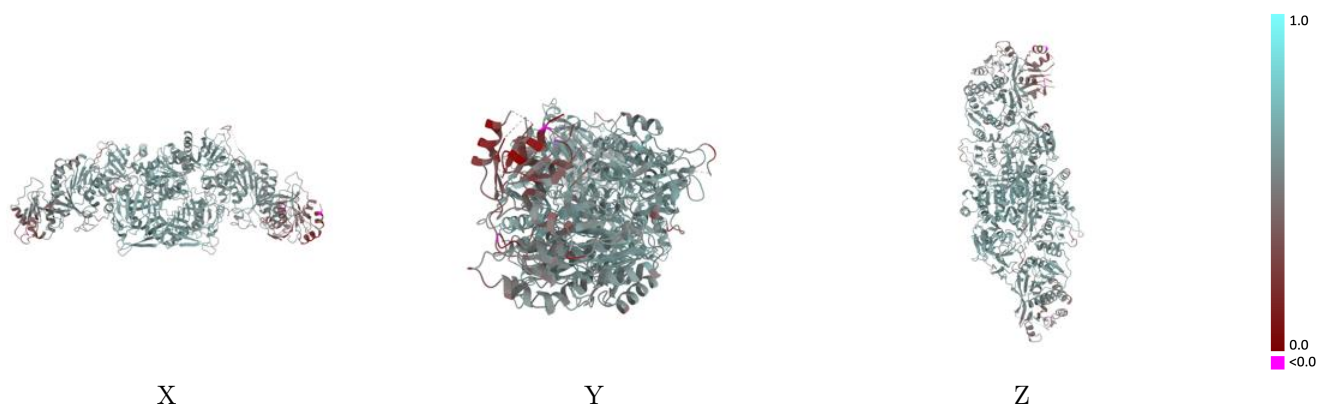
This section contains information regarding the fit between EMDB map EMD-28691 and PDB model 8EYK. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



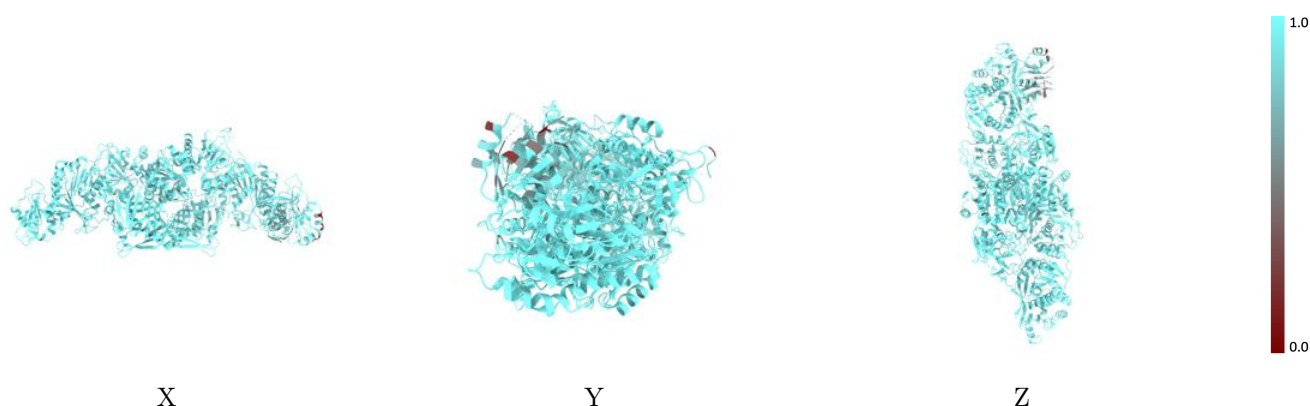
The images above show the 3D surface view of the map at the recommended contour level 0.341 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



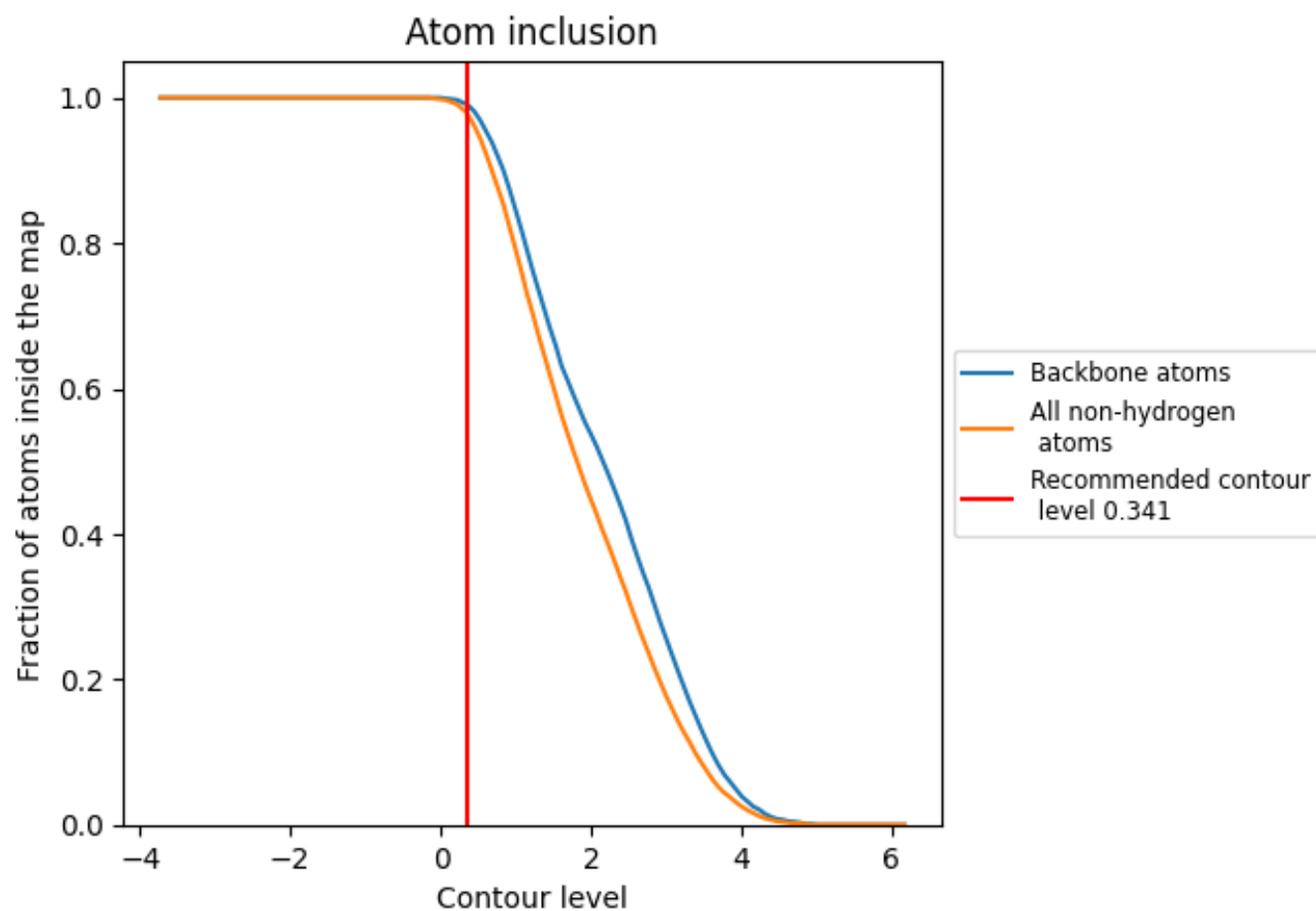
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.341).

9.4 Atom inclusion [i](#)



At the recommended contour level, 99% of all backbone atoms, 98% 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 (0.341) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.9800	<div></div> 0.5550
E	<div></div> 0.9910	<div></div> 0.5690
F	<div></div> 0.9690	<div></div> 0.5420

