



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 06:47 PM UTC

PDB ID : 8YFC / pdb_00008yfc
EMDB ID : EMD-39219
Title : Human PIEZO1-A1988V-MDFIC
Authors : Zhang, M.F.
Deposited on : 2024-02-24
Resolution : 3.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

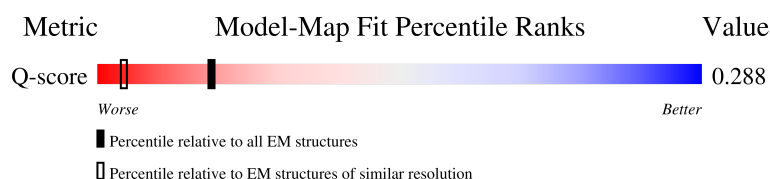
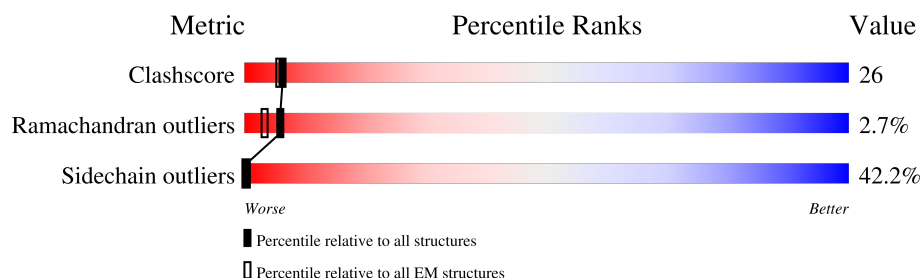
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.20 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	15020 (2.70 - 3.70)

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

Mol	Chain	Length	Quality of chain
1	A	2521	
1	B	2521	
1	D	2521	
2	C	246	

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Mol	Chain	Length	Quality of chain	
2	E	246	 6% ..	91%
2	F	246	 6% ..	91%

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
3	D12	E	301	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 32172 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.

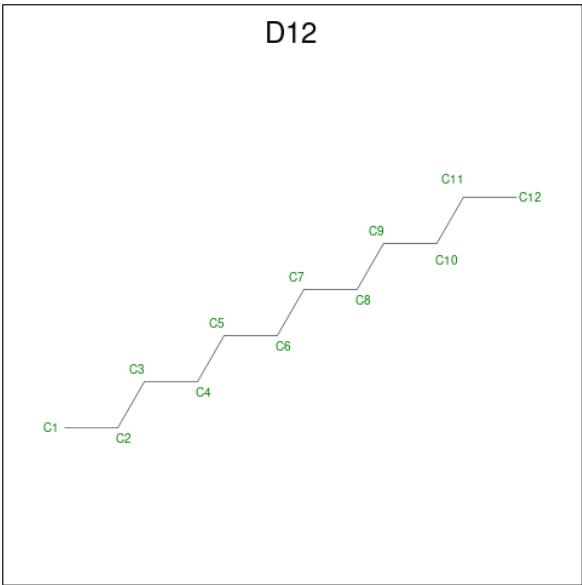
- Molecule 1 is a protein called Piezo-type mechanosensitive ion channel component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1280	Total 10463	C 6920	N 1743	O 1739	S 61	0	0
1	B	1280	Total 10463	C 6920	N 1743	O 1739	S 61	0	0
1	D	1280	Total 10463	C 6920	N 1743	O 1739	S 61	0	0

- Molecule 2 is a protein called MyoD family inhibitor domain-containing protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	21	Total 150	C 88	N 21	O 33	S 8	0	0
2	E	21	Total 150	C 88	N 21	O 33	S 8	0	0
2	F	21	Total 150	C 88	N 21	O 33	S 8	0	0

- Molecule 3 is DODECANE (CCD ID: D12) (formula: C₁₂H₂₆) (labeled as "Ligand of Interest" by depositor).



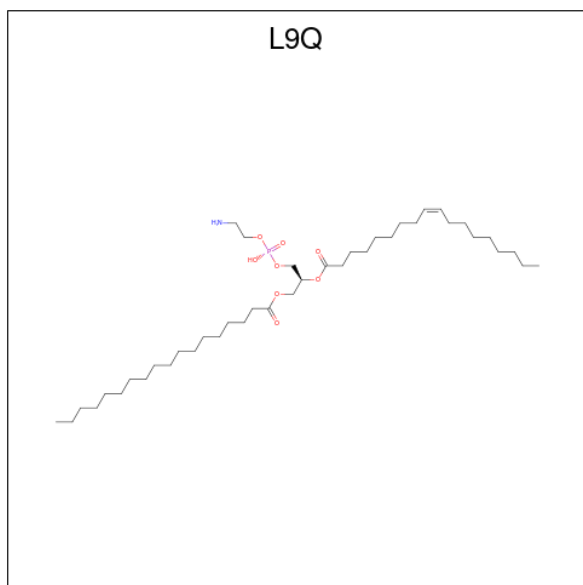
Mol	Chain	Residues	Atoms		AltConf
3	A	1	Total	C	0
			12	12	
3	A	1	Total	C	0
			12	12	
3	B	1	Total	C	0
			12	12	
3	B	1	Total	C	0
			12	12	
3	D	1	Total	C	0
			12	12	
3	D	1	Total	C	0
			12	12	
3	C	1	Total	C	0
			12	12	
3	C	1	Total	C	0
			12	12	
3	C	1	Total	C	0
			12	12	
3	E	1	Total	C	0
			12	12	
3	E	1	Total	C	0
			12	12	
3	E	1	Total	C	0
			12	12	
3	F	1	Total	C	0
			12	12	
3	F	1	Total	C	0
			12	12	

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Mol	Chain	Residues	Atoms	AltConf
3	F	1	Total C 12 12	0

- Molecule 4 is (1S)-2-[[[(S)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-1-[(octadecanoyloxymethyl)ethyl (9Z)-octadec-9-enoate (CCD ID: L9Q) (formula: C₄₁H₈₀NO₈P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C N O P 51 41 1 8 1	0
4	B	1	Total C N O P 51 41 1 8 1	0
4	D	1	Total C N O P 51 41 1 8 1	0



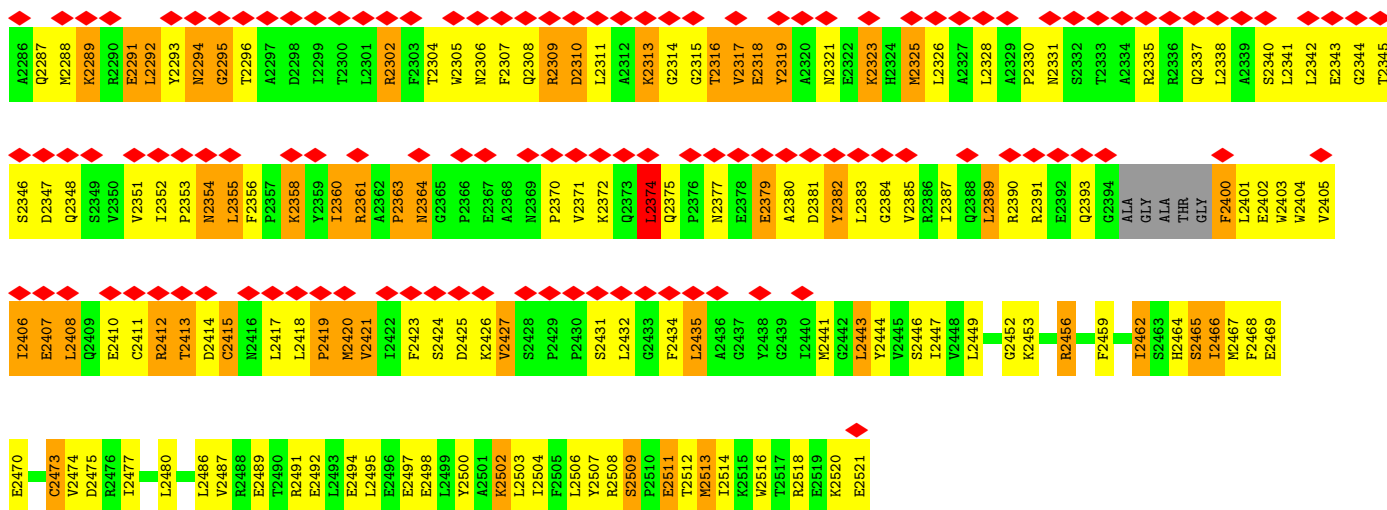






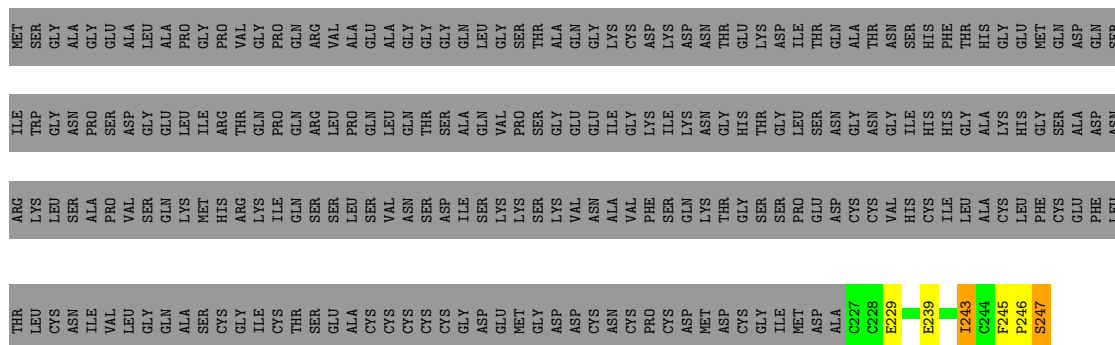


S2226	K2157	T2081	Q1999	GLY	ARG	GLY	ARG	ASP	THR	ARG	THR	ASP	LEU	GLY	T1737	H1536	GLN	GLU	I1336
A2227	K2158	R2082	V2000	ARG	ARG	ARG	ARG	THR	ARG	THR	ARG	ASP	LEU	GLY	E1739	H1536	TRP	GLN	R1340
Q2228	Q2159	C2083	P2001	LEU	GLN	GLN	GLN	ARG	GLY	GLY	GLY	ASP	GLY	GLY	V1741	M1539	TRP	ARG	E1343
Q2229	Q2160	V2085	A2003	GLY	GLY	GLY	GLY	ILE	GLY	GLY	GLY	GLY	GLY	GLY	E1660	D1541	LEU	GLN	E1344
P2230	Q2161	P2086	F2004	PHE	PHE	PHE	PHE	SER	SER	SER	SER	SER	SER	SER	E1662	V1542	TRP	GLN	K1345
I2232	K2163	T2087	F2005	CYS	CYS	CYS	CYS	LEU	LEU	LEU	LEU	LEU	LEU	LEU	Y1745	L1543	PRO	ALA	S1346
I2233	K2088	R2088	L2006	LEU	LEU	LEU	LEU	ARG	ARG	ARG	ARG	ARG	ARG	ARG	E1663	R1544	LEU	GLY	L1347
P2234	K2164	L2089	M2007	SER	SER	SER	SER	PHE	PHE	PHE	PHE	PHE	PHE	PHE	L1746	A1545	ASP	GLN	A1348
F2235	K2165	L2090	L2008	LEU	LEU	LEU	LEU	ARG	ARG	ARG	ARG	ARG	ARG	ARG	F1747	E1546	LEU	PRO	Q1349
F2236	K2167	L2094	L2009	ALA	ALA	ALA	ALA	ARG	ARG	ARG	ARG	ARG	ARG	ARG	GLN	E1547	THR	GLY	L1350
T2237	K2168	T2095	L2010	GLN	GLN	GLN	GLN	ARG	ARG	ARG	ARG	ARG	ARG	ARG	A1666	Y1548	GLY	GLY	K1351
A2237	K2169	K2096	Q2011	GLY	GLY	GLY	GLY	LYS	LYS	LYS	LYS	LYS	LYS	LYS	Q1667	L1549	GLY	GLY	
Q2238	I2170	K2097	F2012	THR	THR	THR	THR	LYS	LYS	LYS	LYS	LYS	LYS	LYS	Q1668	L1550	GLY	GLY	
A2239	V2171	Y2098	M2015	THR	THR	THR	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	E1672	L1551	PRO	GLY	
Y2240	K2172	Y2099	V2016	ARG	ARG	ARG	ARG	PRO	PRO	PRO	PRO	PRO	PRO	PRO	L1673	Q1552	PRO	GLY	S1423
F2241	M2175	L2101	R2019	P1940	P1941	P1942	P1943	ALA	ALA	ALA	ALA	ALA	ALA	ALA	R1674	T1552	GLY	GLY	D1424
E2242		L2102	L2023	R1944	R1945	R1946	R1947	ARG	ARG	ARG	ARG	ARG	ARG	ARG	L1675	R1553	GLY	GLY	A1425
L2243	I2184	L2103	R2024	L1949	L1950	L1951	L1952	ILE	ILE	ILE	ILE	ILE	ILE	ILE	L1676	L1554	VAL	VAL	E1426
E2244	A2185	F2104	T2025	L1953	L1954	L1955	L1956	GLY	GLY	GLY	GLY	GLY	GLY	GLY	R1677	L1555	GLY	GLY	E1427
R2245	I2187	L2105	V2027	R1953	R1954	R1955	R1956	GLY	GLY	GLY	GLY	GLY	GLY	GLY	Q1681	Q1556	GLY	GLY	
Q2246	F2188	L2106	L2028	L1953	L1954	L1955	L1956	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1687	G1558	ALA	ALA	
F2247	P2190	Q2107	G2028	R1953	R1954	R1955	R1956	GLY	GLY	GLY	GLY	GLY	GLY	GLY	E1688	V1560	GLY	GLY	
D2248	L2191	R2110	K2030	L1953	L1954	L1955	L1956	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1689	H1561	PRO	GLY	
P2249	F2193	L2111	L2031	R1953	R1954	R1955	R1956	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1690	R1562	GLY	GLY	
Q2250	M2194	R2112	L2031	R1953	R1954	R1955	R1956	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1691	G1563	ALA	ALA	
P2251	R2198	F2114	L2037	T1968	T1969	T1970	T1971	ARG	ARG	ARG	ARG	ARG	ARG	ARG	L1692	V1564	PRO	PRO	
L2252	S2199	L2115	L2037	D1968	D1969	D1970	D1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1693	L1565	ALA	ALA	
A2253	V2200	V2116	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	H1697	D1566	GLY	GLY	
M2254	V2201	V2117	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	Q1567	Q1567	ALA	ALA	
Q2255	V2202	V2118	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1568	L1568	GLY	GLY	
I2257	V2203	V2119	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	TYR	TYR	THR	THR	
S2258	V2204	V2120	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	A1703	A1703	VAL	VAL	
Q2259	V2205	V2121	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	S1704	S1704	ALA	ALA	
Y2260	V2206	V2122	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	A1705	A1705	GLY	GLY	
S2261	V2207	V2123	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	G1706	G1706	GLY	GLY	
P2262	I2208	V2124	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	S1707	S1707	ALA	ALA	
E2263	D2209	S2135	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	G1708	G1708	GLY	GLY	
D2264	V2210	S2136	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1709	L1709	ALA	ALA	
I2265	V2211	M2137	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	V1709	V1709	THR	THR	
V2266	T2212	E2140	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	L1710	L1710	GLY	GLY	
T2267	V2213	L2146	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	V1714	V1714	PRO	PRO	
A2268	L2214	F2147	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	F1715	F1715	GLY	GLY	
Q2269	K2215	K2150	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	M1719	M1719	GLY	GLY	
L2270	L2216	C2151	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	I1722	I1722	THR	THR	
E2271	G2217	S2152	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	P1723	P1723	ALA	ALA	
G2272	G2218	R2153	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	R1724	R1724	GLY	GLY	
S2273	Y2219	E2154	L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	P1725	P1725	ASN	ASN	
S2274	E2220		L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	S1726	S1726	ALA	ALA	
Q2275	P2221		L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	K1727	K1727	PRO	PRO	
A2276	L2222		L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	R1728	R1728	THR	THR	
L2277	F2223		L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	M1731	M1731	VAL	VAL	
W2278	R2279		L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	T1732	T1732	SER	SER	
R2279	L2280		L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	M1733	M1733	GLY	GLY	
L2280	S2281		L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	A1733	A1733	GLY	GLY	
S2281	P2282		L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	R1655	R1655	GLY	GLY	
P2283	S2284		L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	R1655	R1655	GLY	GLY	
S2284	R2285		L2043	V1968	V1969	V1970	V1971	GLY	GLY	GLY	GLY	GLY	GLY	GLY	R1655	R1655	GLY	GLY	



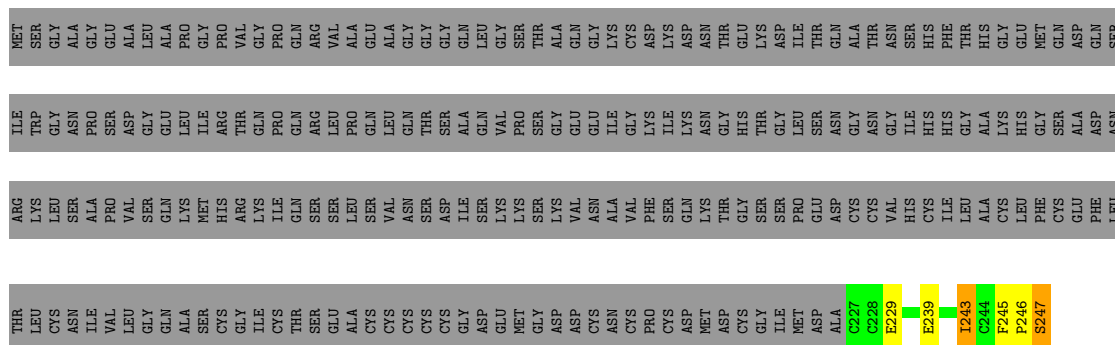
• Molecule 2: MyoD family inhibitor domain-containing protein

Chain C: 6% .. 91%



• Molecule 2: MyoD family inhibitor domain-containing protein

Chain E: 6% .. 91%



• Molecule 2: MyoD family inhibitor domain-containing protein

Chain F: 6% .. 91%



THR	ARG	ILE
LEU	LYS	TRP
CYS	LEU	GLY
ASN	SER	ASN
ILE	ALA	PRO
VAL	PRO	SER
LEU	VAL	ASP
GLY	SER	GLY
GLN	GLN	GLU
ALA	LYS	LEU
ALA	SER	ILE
CYS	HIS	ARG
GLY	ARG	THR
ILE	LYS	GLN
CYS	ILE	PRO
THR	GLN	GLN
SER	SER	ARG
GLU	SER	LEU
ALA	LEU	PRO
CYS	SER	GLN
CYS	VAL	LEU
CYS	ASN	GLN
CYS	SER	THR
CYS	ASP	SER
GLY	ILE	ALA
ASP	SER	GLN
GLU	LYS	VAL
MET	LYS	GLY
ASP	LYS	GLY
ASP	VAL	GLU
CYS	ASN	GLU
ASN	ALA	ILE
CYS	VAL	GLY
PRO	PHE	LYS
CYS	SER	ILE
ASP	GLN	LYS
MET	LYS	ASN
ASP	THR	GLY
CYS	GLY	HIS
GLY	SER	THR
ILE	SER	GLY
MET	PRO	LEU
ASP	GLU	SER
ALA	ASP	ASN
C227	CYS	GLY
C228	CYS	ASN
E229	VAL	GLY
E239	HIS	ILE
E239	CYS	HIS
E239	ILE	HIS
E239	LEU	GLY
I243	ALA	ALA
C244	CYS	LYS
F245	LEU	HIS
P246	PHE	GLY
S247	CYS	SER
	GLU	ALA
	PHE	ASP
	LEU	ASN

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	40207	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TECNAI 10	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.385	Depositor
Minimum map value	-0.227	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.04	Depositor
Map size ($\text{\AA}$)	456.0, 456.0, 456.0	wwPDB
Map dimensions	800, 800, 800	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	0.57, 0.57, 0.57	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: D12, L9Q

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	0.55	2/10719 (0.0%)	0.91	51/14526 (0.4%)
1	B	0.55	2/10719 (0.0%)	0.96	53/14526 (0.4%)
1	D	0.55	2/10719 (0.0%)	0.91	51/14526 (0.4%)
2	C	0.71	0/151	1.16	0/200
2	E	0.71	0/151	1.16	0/200
2	F	0.70	0/151	1.16	0/200
All	All	0.55	6/32610 (0.0%)	0.93	155/44178 (0.4%)

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	1160	VAL	CA-CB	6.03	1.62	1.54
1	A	1160	VAL	CA-CB	6.02	1.62	1.54
1	B	1160	VAL	CA-CB	6.00	1.62	1.54
1	D	2289	LYS	C-N	-5.10	1.27	1.33
1	B	2289	LYS	C-N	-5.09	1.27	1.33

The worst 5 of 155 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	584	CYS	CA-CB-SG	-35.48	29.68	104.20
1	B	930	GLN	N-CA-C	11.20	126.52	113.19
1	A	930	GLN	N-CA-C	11.19	126.51	113.19
1	D	930	GLN	N-CA-C	11.19	126.51	113.19
1	D	2374	LEU	N-CA-C	-10.05	100.31	111.07

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	10463	0	10689	610	0
1	B	10463	0	10689	603	0
1	D	10463	0	10689	603	0
2	C	150	0	132	11	0
2	E	150	0	132	12	0
2	F	150	0	132	11	0
3	A	24	0	52	3	0
3	B	24	0	52	4	0
3	C	36	0	78	8	0
3	D	24	0	52	4	0
3	E	36	0	78	10	0
3	F	36	0	78	8	0
4	A	51	0	79	8	0
4	B	51	0	79	9	0
4	D	51	0	79	8	0
All	All	32172	0	33090	1679	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 26.

The worst 5 of 1679 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:2459:PHE:CD1	1:D:2137:MET:HE2	1.54	1.42
1:B:2137:MET:HE2	1:D:2459:PHE:CD1	1.54	1.39
1:D:1650:LEU:CD2	1:D:1654:LEU:HD12	1.53	1.39
1:A:2137:MET:HE2	1:B:2459:PHE:CD1	1.54	1.38
1:B:1650:LEU:CD2	1:B:1654:LEU:HD12	1.53	1.38

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	1248/2521 (50%)	1069 (86%)	145 (12%)	34 (3%)	4	25
1	B	1248/2521 (50%)	1069 (86%)	145 (12%)	34 (3%)	4	25
1	D	1248/2521 (50%)	1069 (86%)	145 (12%)	34 (3%)	4	25
2	C	19/246 (8%)	17 (90%)	2 (10%)	0	100	100
2	E	19/246 (8%)	17 (90%)	2 (10%)	0	100	100
2	F	19/246 (8%)	17 (90%)	2 (10%)	0	100	100
All	All	3801/8301 (46%)	3258 (86%)	441 (12%)	102 (3%)	6	25

5 of 102 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1723	PRO
1	A	1725	PRO
1	A	1953	LYS
1	A	2316	THR
1	A	2379	GLU

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	1121/2172 (52%)	642 (57%)	479 (43%)	0	0
1	B	1121/2172 (52%)	642 (57%)	479 (43%)	0	0
1	D	1121/2172 (52%)	642 (57%)	479 (43%)	0	0

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	C	20/203 (10%)	17 (85%)	3 (15%)	3	15
2	E	20/203 (10%)	17 (85%)	3 (15%)	3	15
2	F	20/203 (10%)	17 (85%)	3 (15%)	3	15
All	All	3423/7125 (48%)	1977 (58%)	1446 (42%)	0	0

5 of 1446 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	2431	SER
1	D	1336	ILE
1	B	2512	THR
1	B	2427	VAL
1	D	856	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 65 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	2080	GLN
1	D	2161	GLN
1	B	851	GLN
1	B	702	HIS
1	D	2229	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

18 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
3	D12	A	2601	-	11,11,11	0.26	0	10,10,10	0.42	0
3	D12	D	2603	-	11,11,11	0.27	0	10,10,10	0.39	0
3	D12	C	301	-	11,11,11	0.30	0	10,10,10	0.40	0
3	D12	F	303	-	11,11,11	0.29	0	10,10,10	0.35	0
3	D12	C	303	-	11,11,11	0.29	0	10,10,10	0.35	0
4	L9Q	B	2601	-	50,50,50	1.06	3 (6%)	53,55,55	1.08	3 (5%)
3	D12	B	2602	-	11,11,11	0.26	0	10,10,10	0.42	0
3	D12	C	302	-	11,11,11	0.26	0	10,10,10	0.45	0
4	L9Q	D	2601	-	50,50,50	1.06	3 (6%)	53,55,55	1.08	3 (5%)
3	D12	E	302	-	11,11,11	0.26	0	10,10,10	0.45	0
3	D12	E	303	-	11,11,11	0.29	0	10,10,10	0.35	0
4	L9Q	A	2603	-	50,50,50	1.06	3 (6%)	53,55,55	1.08	3 (5%)
3	D12	D	2602	-	11,11,11	0.26	0	10,10,10	0.42	0
3	D12	A	2602	-	11,11,11	0.27	0	10,10,10	0.39	0
3	D12	F	302	-	11,11,11	0.26	0	10,10,10	0.45	0
3	D12	F	301	-	11,11,11	0.30	0	10,10,10	0.40	0
3	D12	B	2603	-	11,11,11	0.27	0	10,10,10	0.39	0
3	D12	E	301	-	11,11,11	0.29	0	10,10,10	0.40	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
3	D12	A	2601	-	-	7/9/9/9	-
3	D12	D	2603	-	-	6/9/9/9	-
3	D12	C	301	-	-	7/9/9/9	-
3	D12	F	303	-	-	5/9/9/9	-
3	D12	C	303	-	-	5/9/9/9	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	L9Q	B	2601	-	-	30/54/54/54	-
3	D12	B	2602	-	-	7/9/9/9	-
3	D12	C	302	-	-	8/9/9/9	-
4	L9Q	D	2601	-	-	30/54/54/54	-
3	D12	E	302	-	-	8/9/9/9	-
3	D12	E	303	-	-	5/9/9/9	-
4	L9Q	A	2603	-	-	30/54/54/54	-
3	D12	D	2602	-	-	7/9/9/9	-
3	D12	A	2602	-	-	6/9/9/9	-
3	D12	F	302	-	-	8/9/9/9	-
3	D12	F	301	-	-	7/9/9/9	-
3	D12	B	2603	-	-	6/9/9/9	-
3	D12	E	301	-	-	7/9/9/9	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2603	L9Q	O3-C11	4.24	1.45	1.33
4	B	2601	L9Q	O3-C11	4.23	1.45	1.33
4	D	2601	L9Q	O3-C11	4.23	1.45	1.33
4	B	2601	L9Q	O2-C31	4.05	1.45	1.34
4	A	2603	L9Q	O2-C31	4.05	1.45	1.34

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	2601	L9Q	O2-C31-C32	3.86	119.82	111.48
4	D	2601	L9Q	O2-C31-C32	3.85	119.81	111.48
4	A	2603	L9Q	O2-C31-C32	3.84	119.80	111.48
4	D	2601	L9Q	O3-C11-C12	2.85	120.51	111.83
4	A	2603	L9Q	O3-C11-C12	2.84	120.50	111.83

There are no chirality outliers.

5 of 189 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2603	L9Q	C1-O3P-P-O1P
4	A	2603	L9Q	C1-O3P-P-O2P

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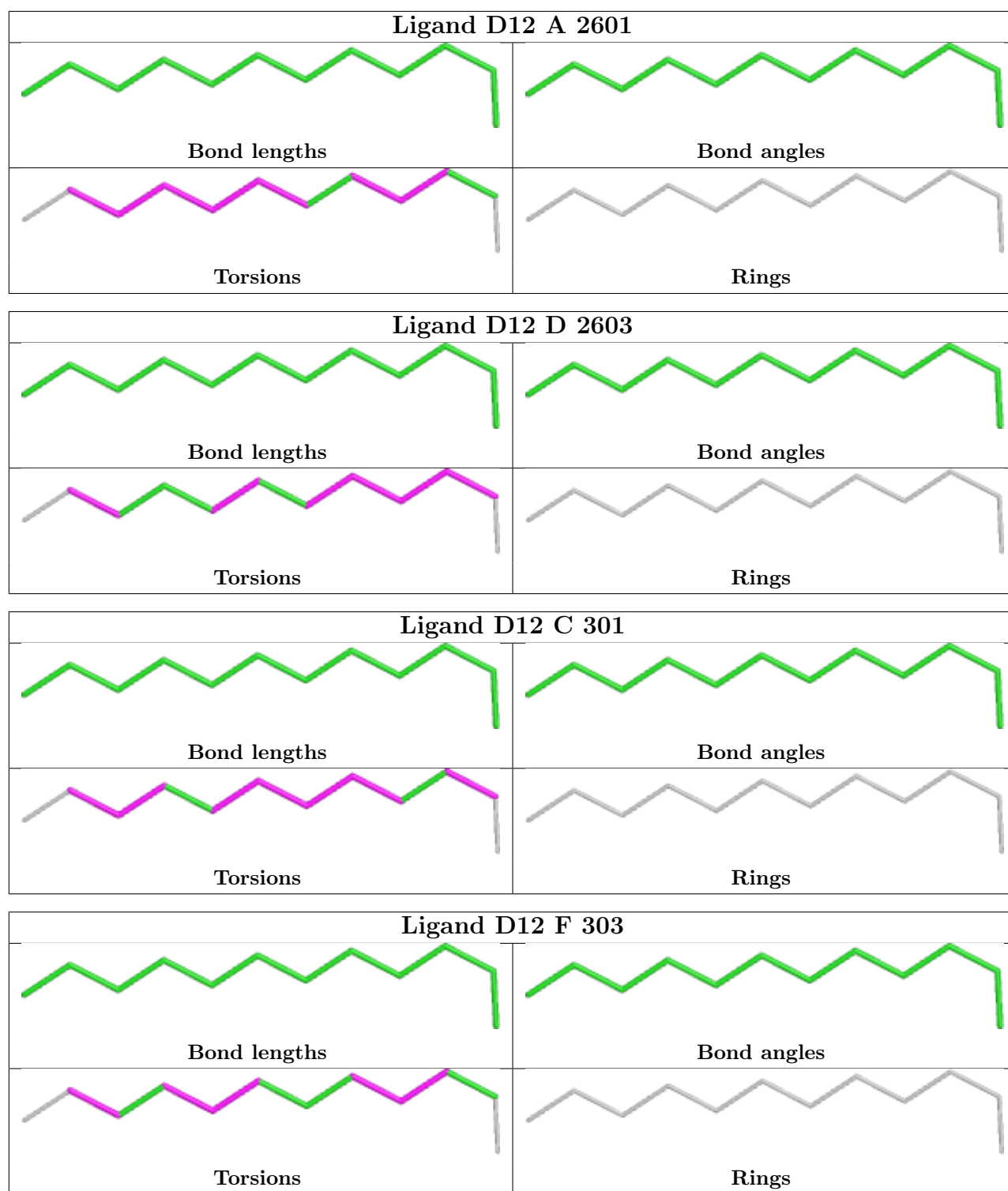
Mol	Chain	Res	Type	Atoms
4	A	2603	L9Q	C1-O3P-P-O4P
4	A	2603	L9Q	O4P-C4-C5-N
4	B	2601	L9Q	C1-O3P-P-O1P

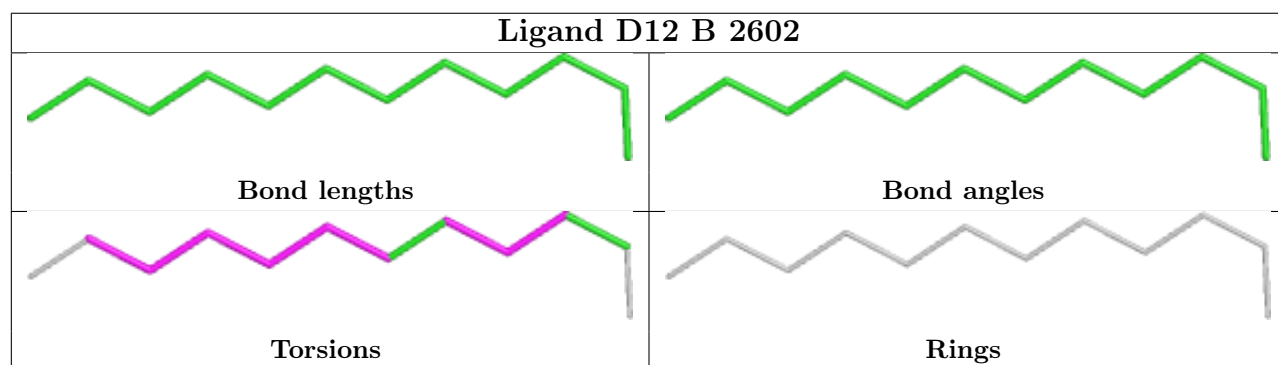
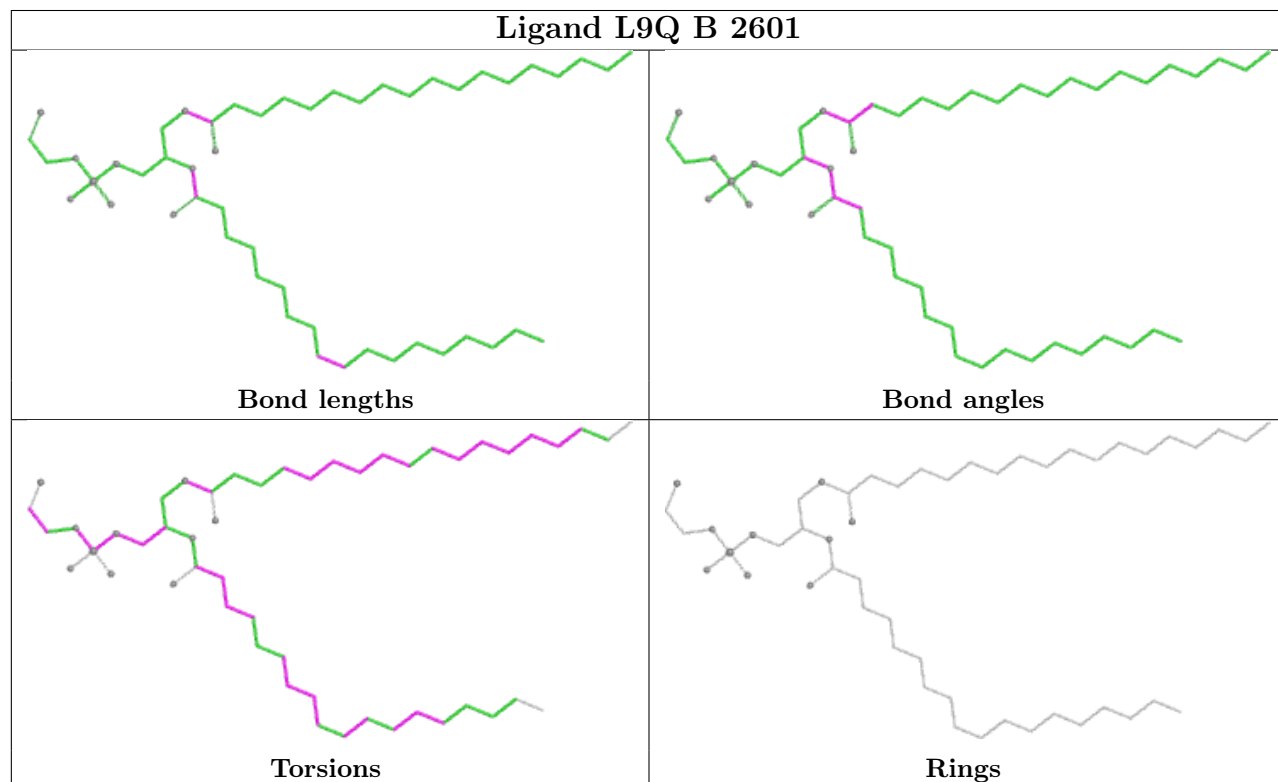
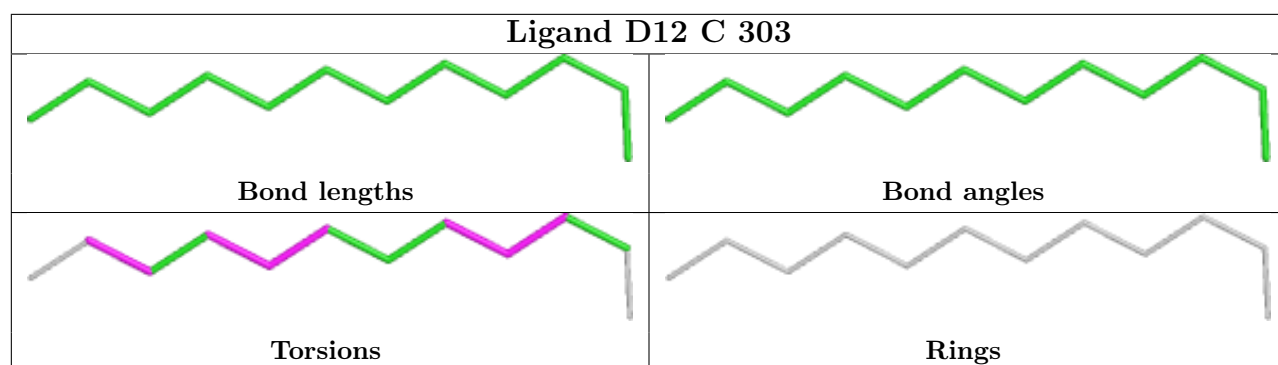
There are no ring outliers.

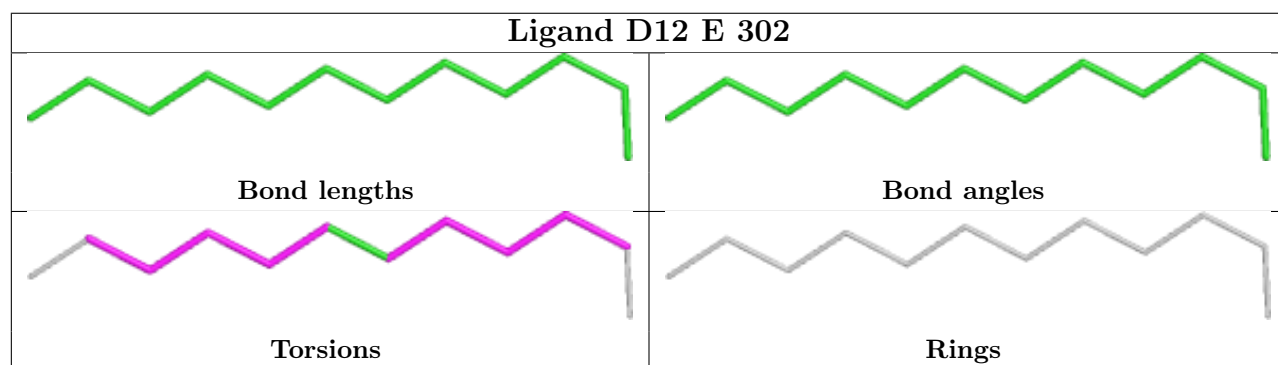
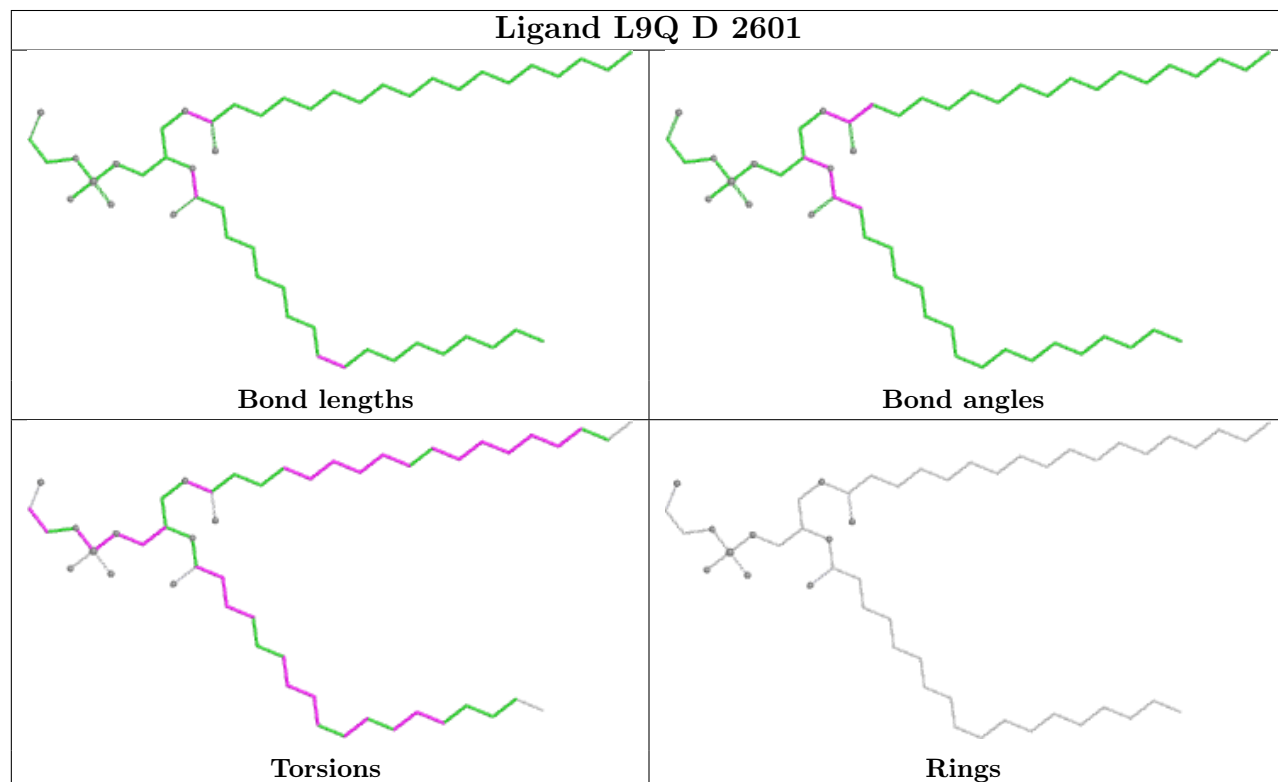
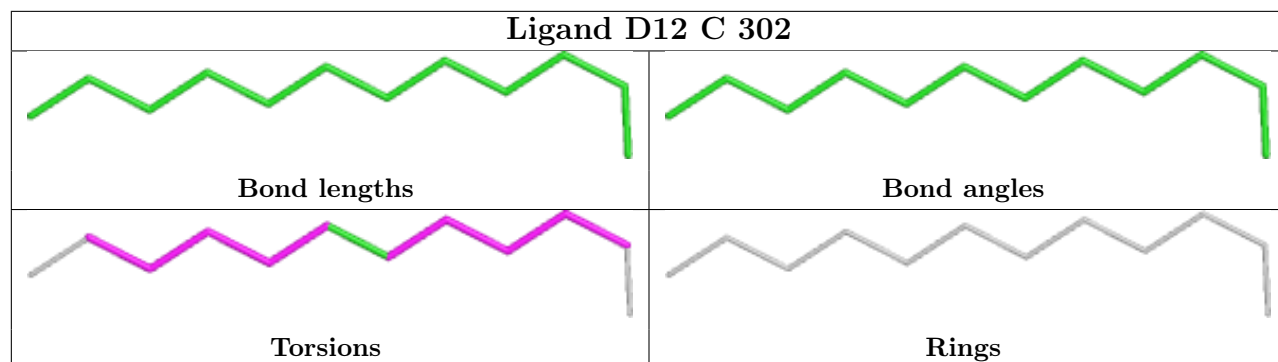
18 monomers are involved in 53 short contacts:

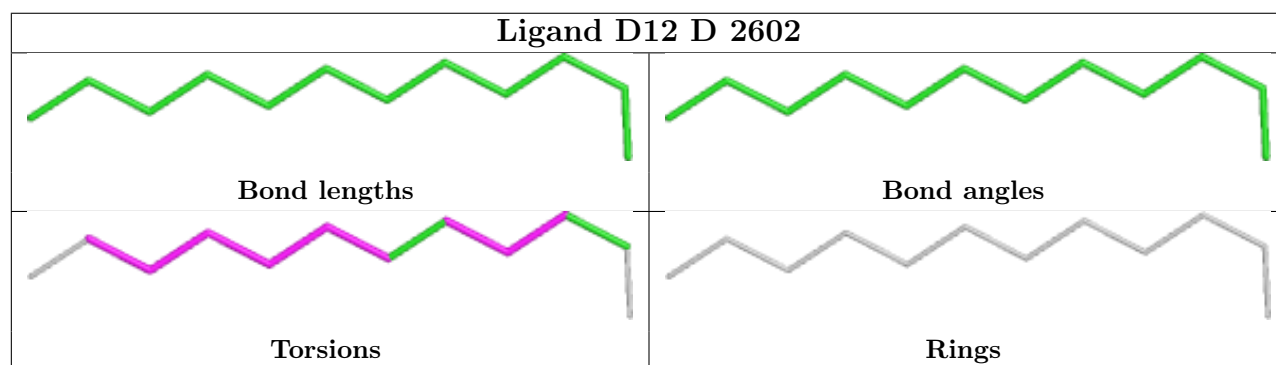
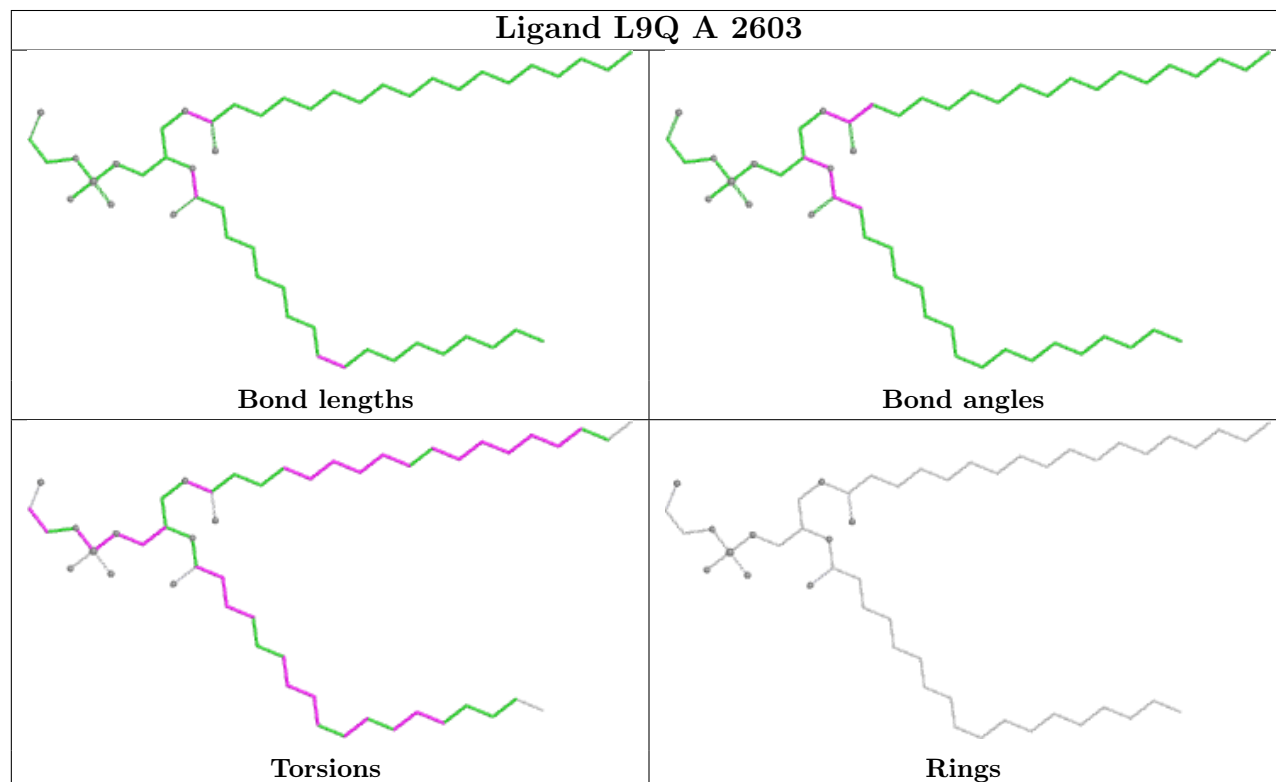
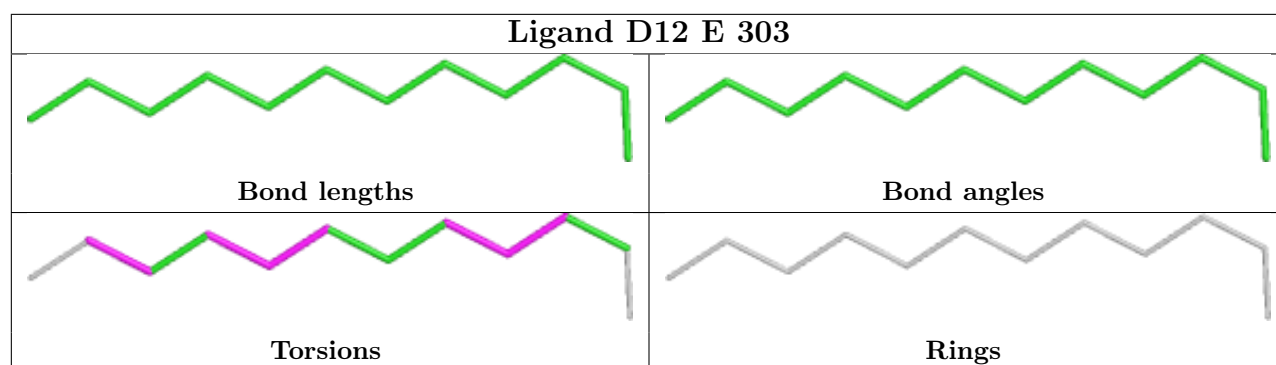
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2601	D12	1	0
3	D	2603	D12	2	0
3	C	301	D12	5	0
3	F	303	D12	3	0
3	C	303	D12	3	0
4	B	2601	L9Q	9	0
3	B	2602	D12	2	0
3	C	302	D12	2	0
4	D	2601	L9Q	8	0
3	E	302	D12	2	0
3	E	303	D12	3	0
4	A	2603	L9Q	8	0
3	D	2602	D12	2	0
3	A	2602	D12	2	0
3	F	302	D12	2	0
3	F	301	D12	5	0
3	B	2603	D12	2	0
3	E	301	D12	7	0

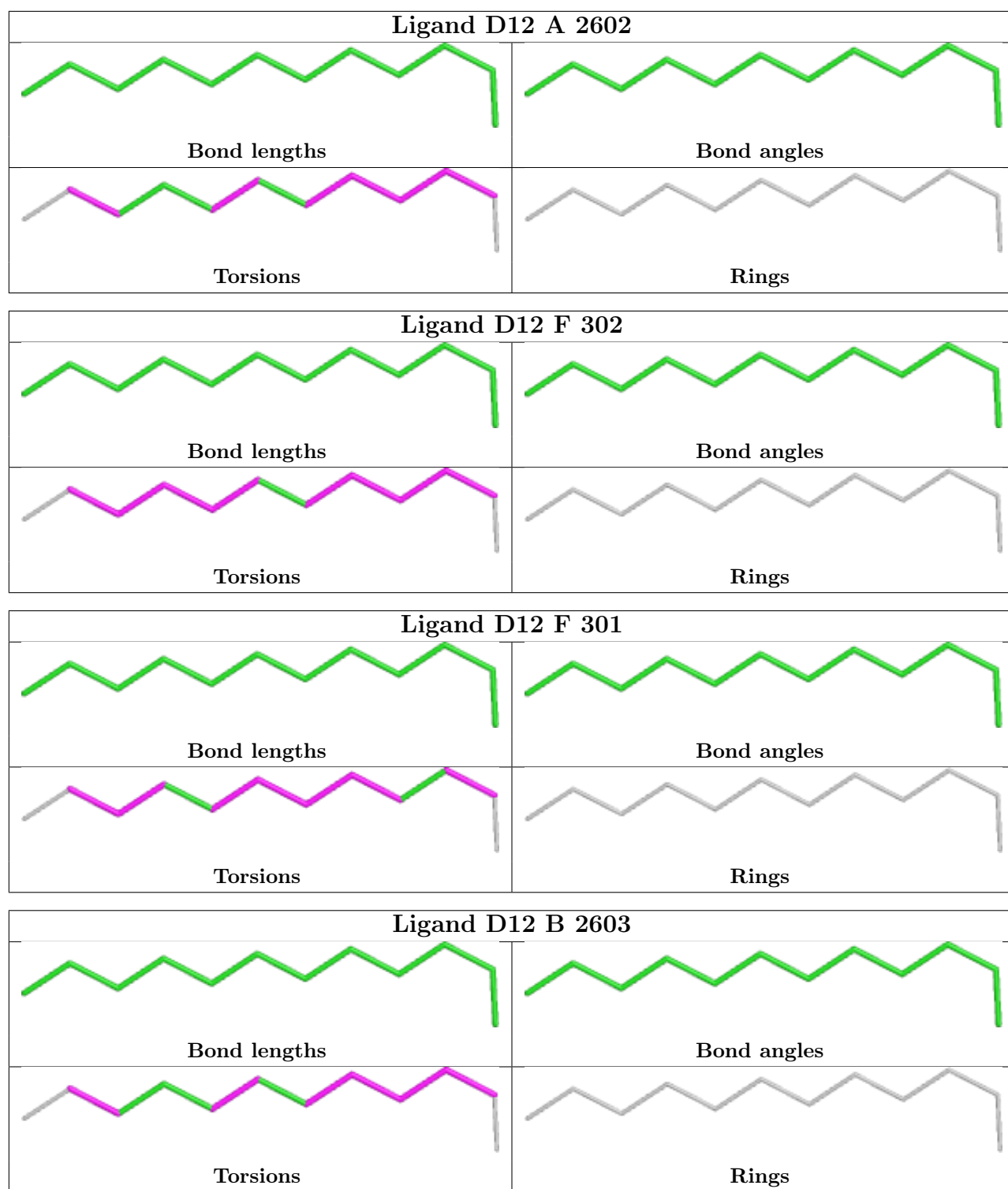
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

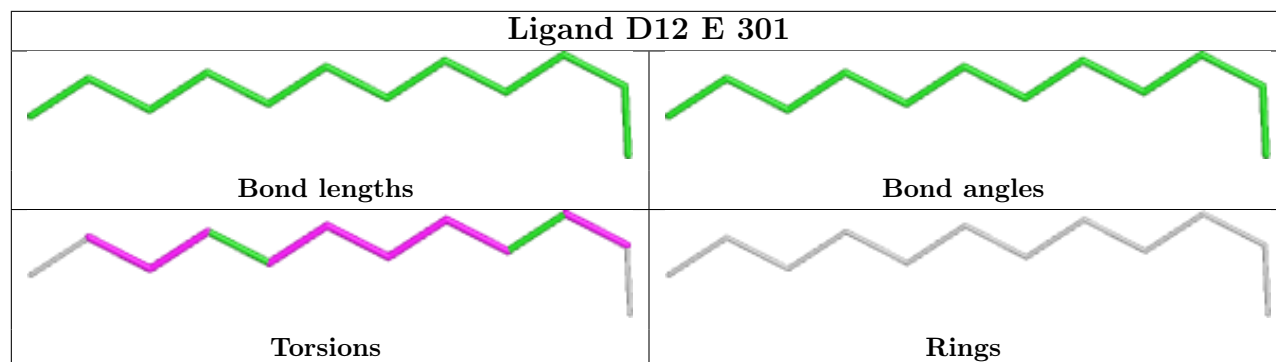












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

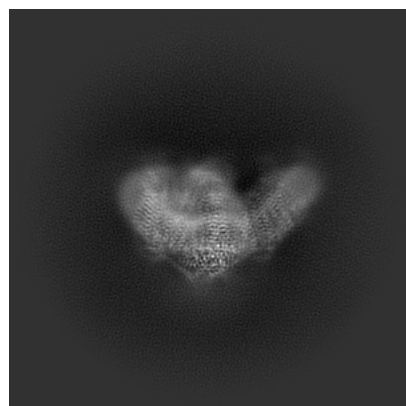
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-39219. These allow visual inspection of the internal detail of the map and identification of artifacts.

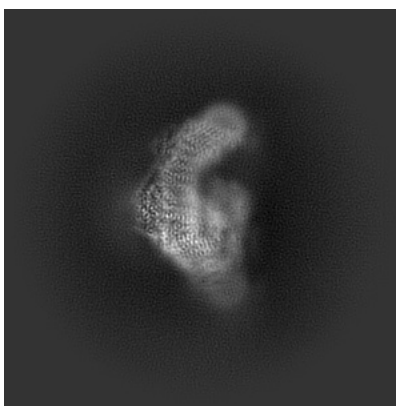
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

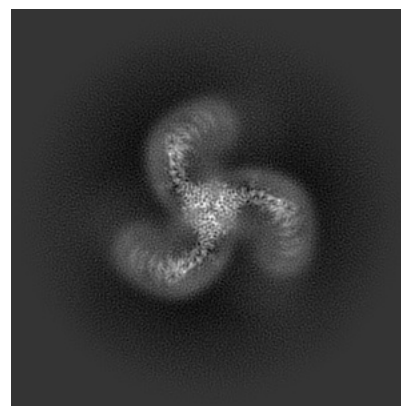
6.1.1 Primary map



X

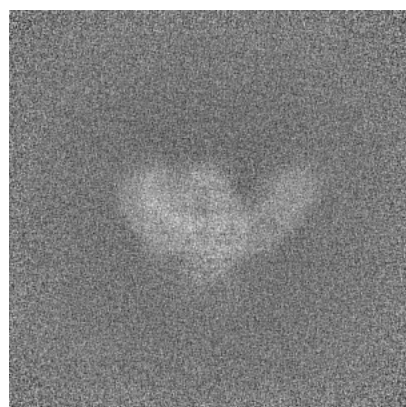


Y

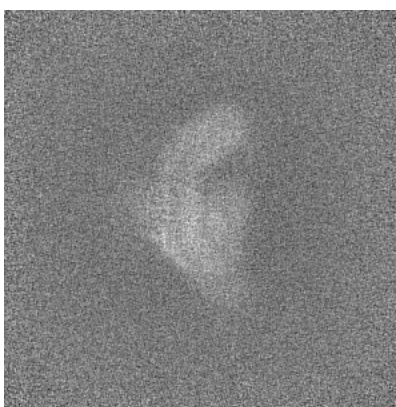


Z

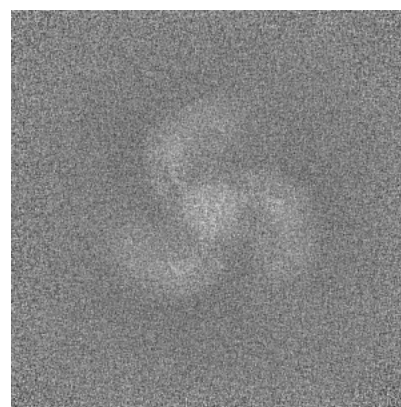
6.1.2 Raw map



X



Y



Z

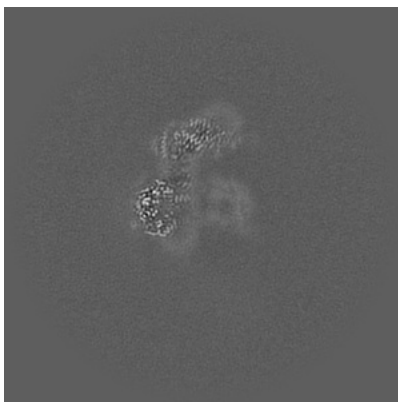
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

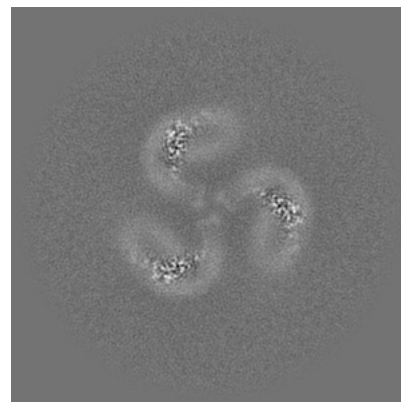
6.2.1 Primary map



X Index: 400

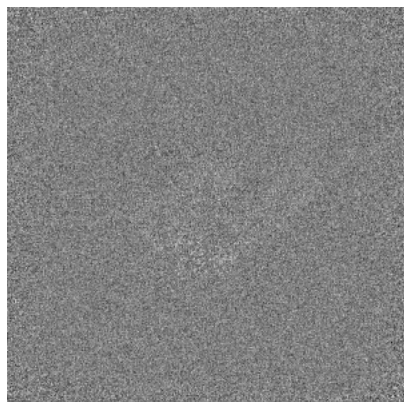


Y Index: 400

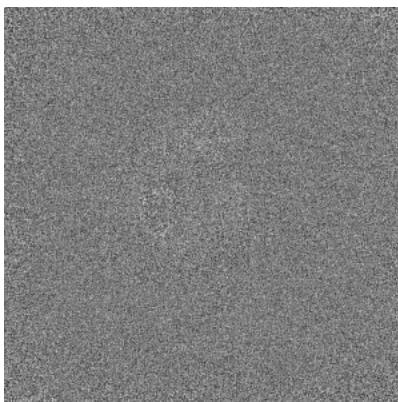


Z Index: 400

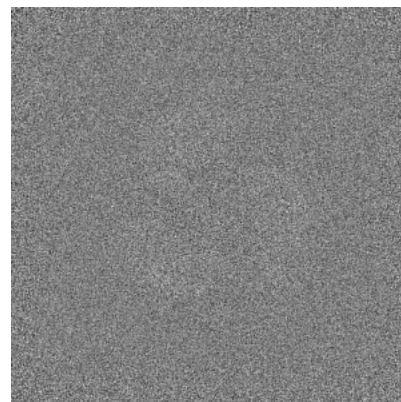
6.2.2 Raw map



X Index: 400



Y Index: 400

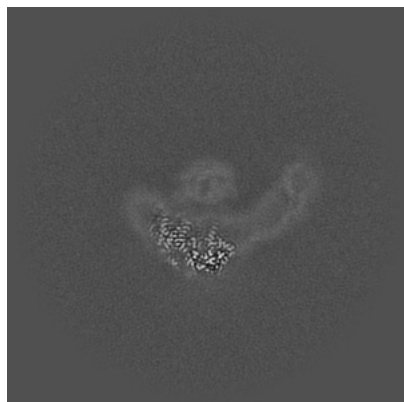


Z Index: 400

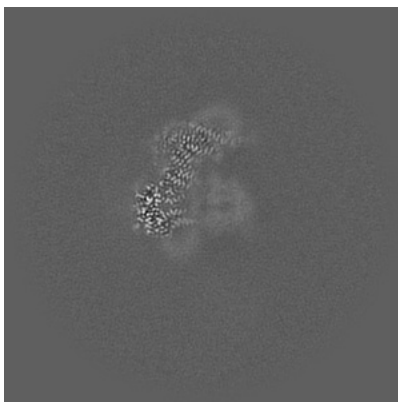
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

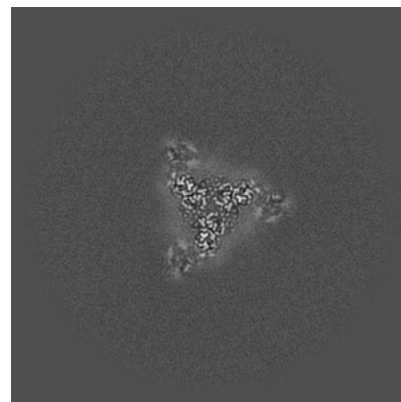
6.3.1 Primary map



X Index: 386

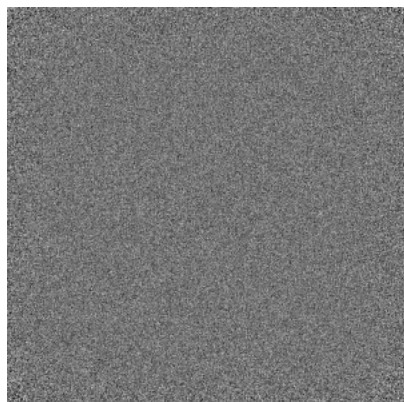


Y Index: 409

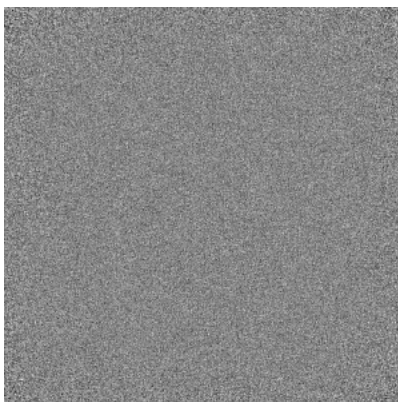


Z Index: 326

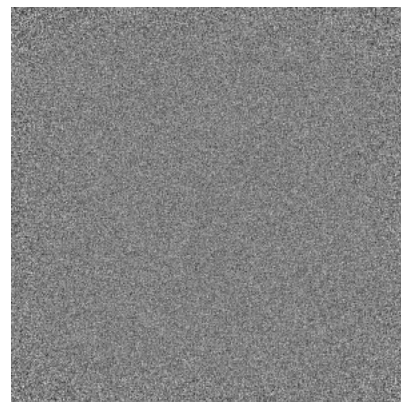
6.3.2 Raw map



X Index: 0



Y Index: 0



Z Index: 0

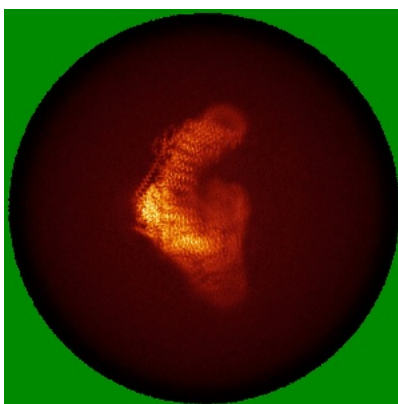
The images above show the largest variance slices of the map in three orthogonal directions.

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

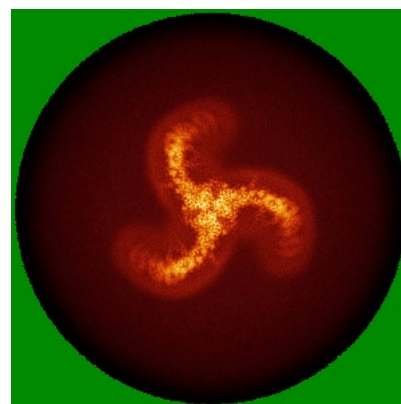
6.4.1 Primary map



X

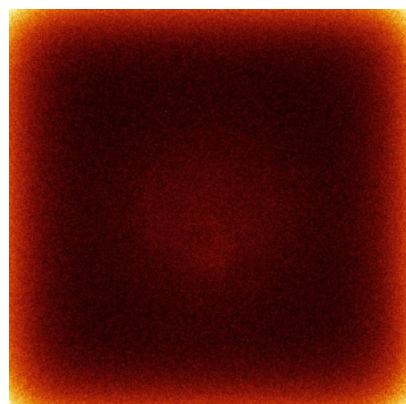


Y

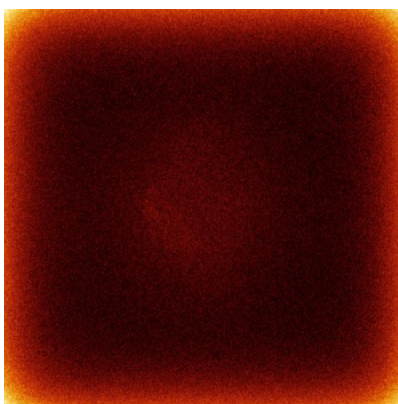


Z

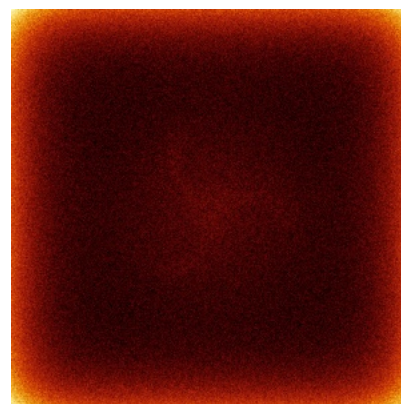
6.4.2 Raw map



X



Y

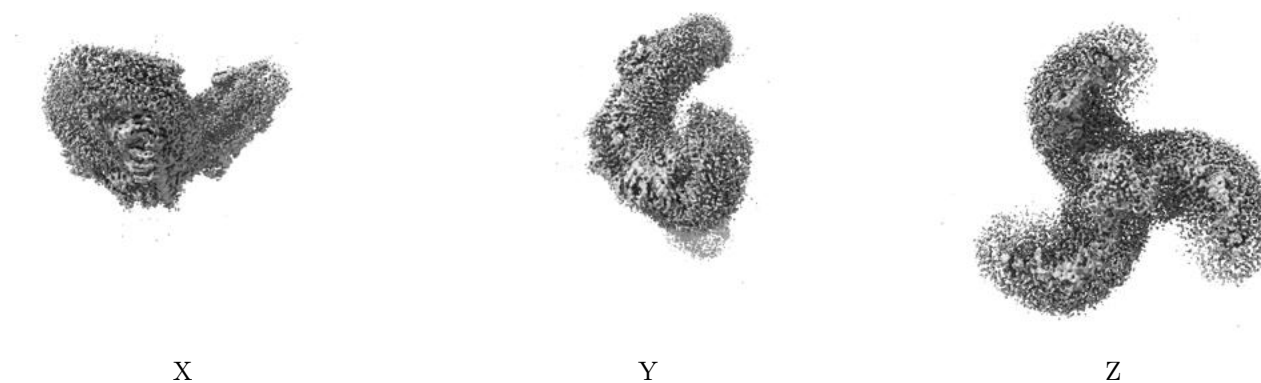


Z

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.

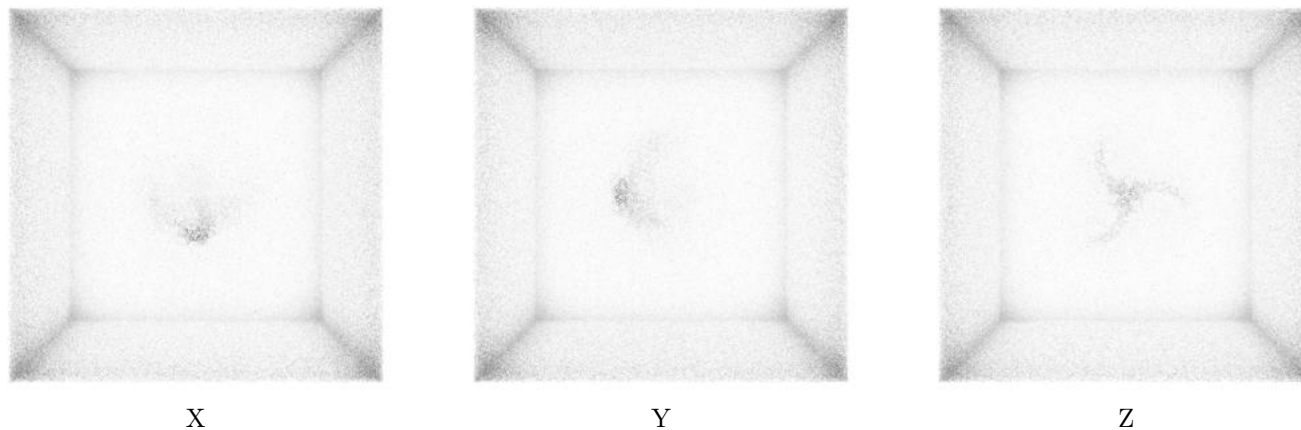
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.04. 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.

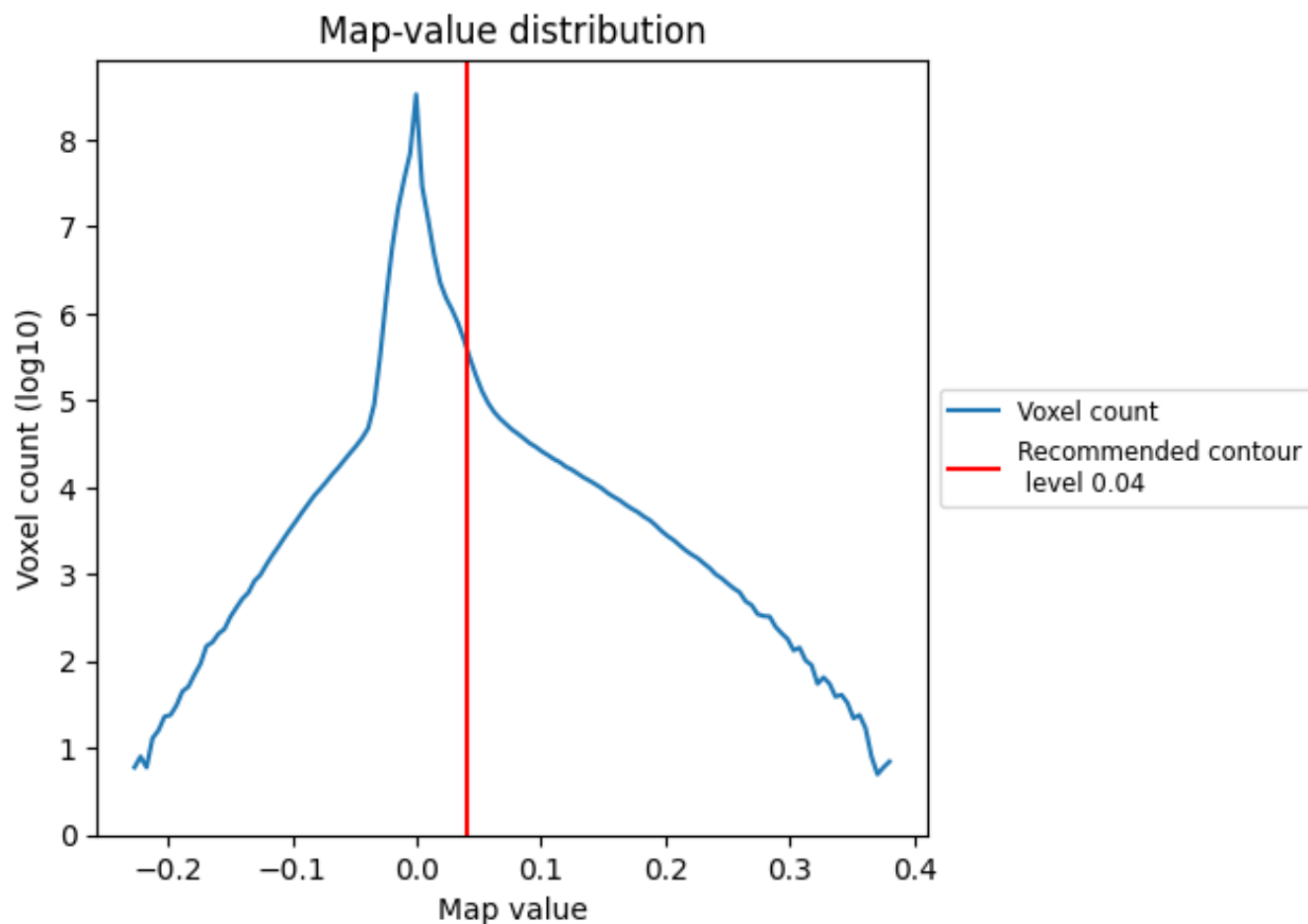
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

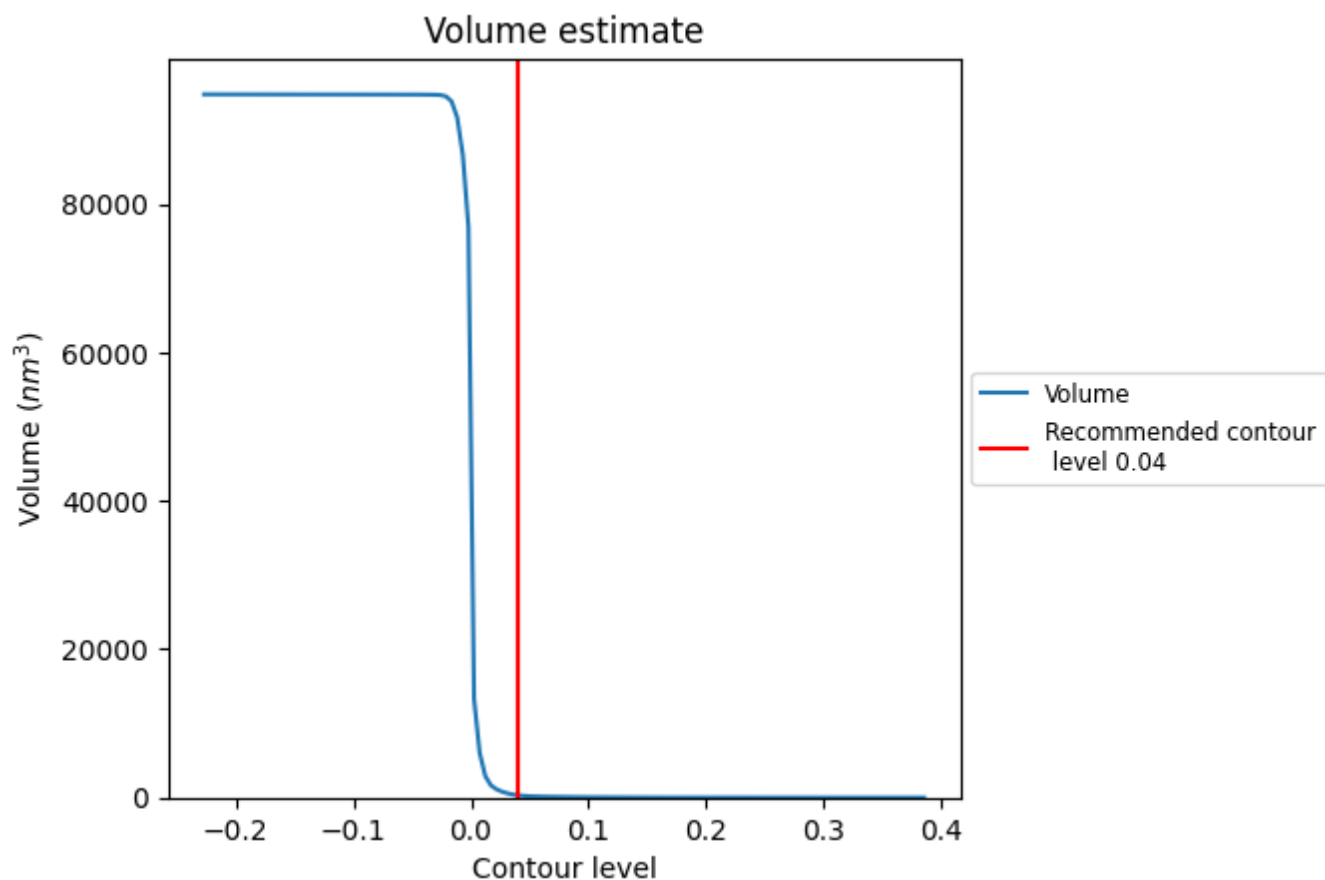
This section contains the results of statistical analysis of the map.

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.

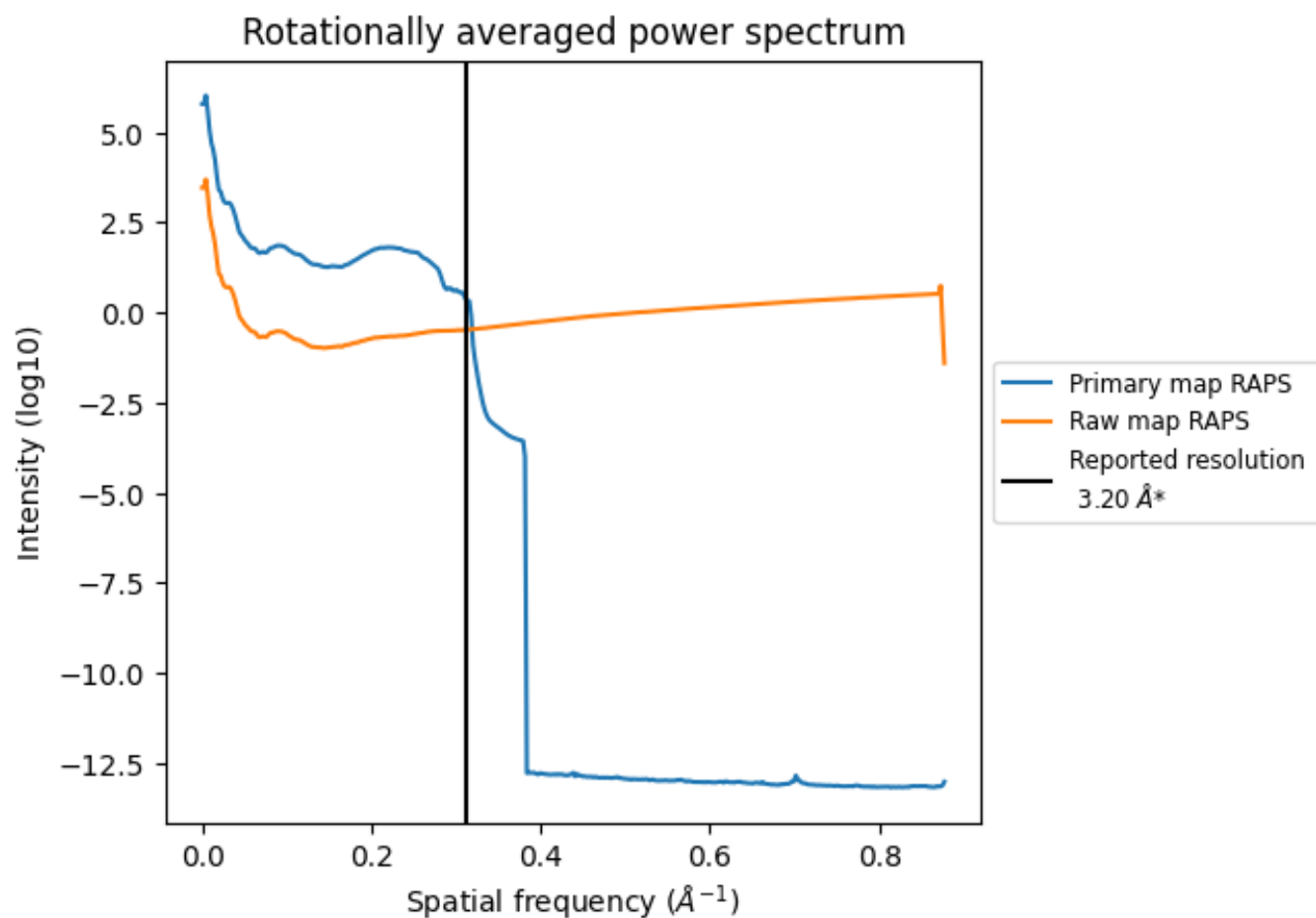
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 304 nm³; this corresponds to an approximate mass of 275 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

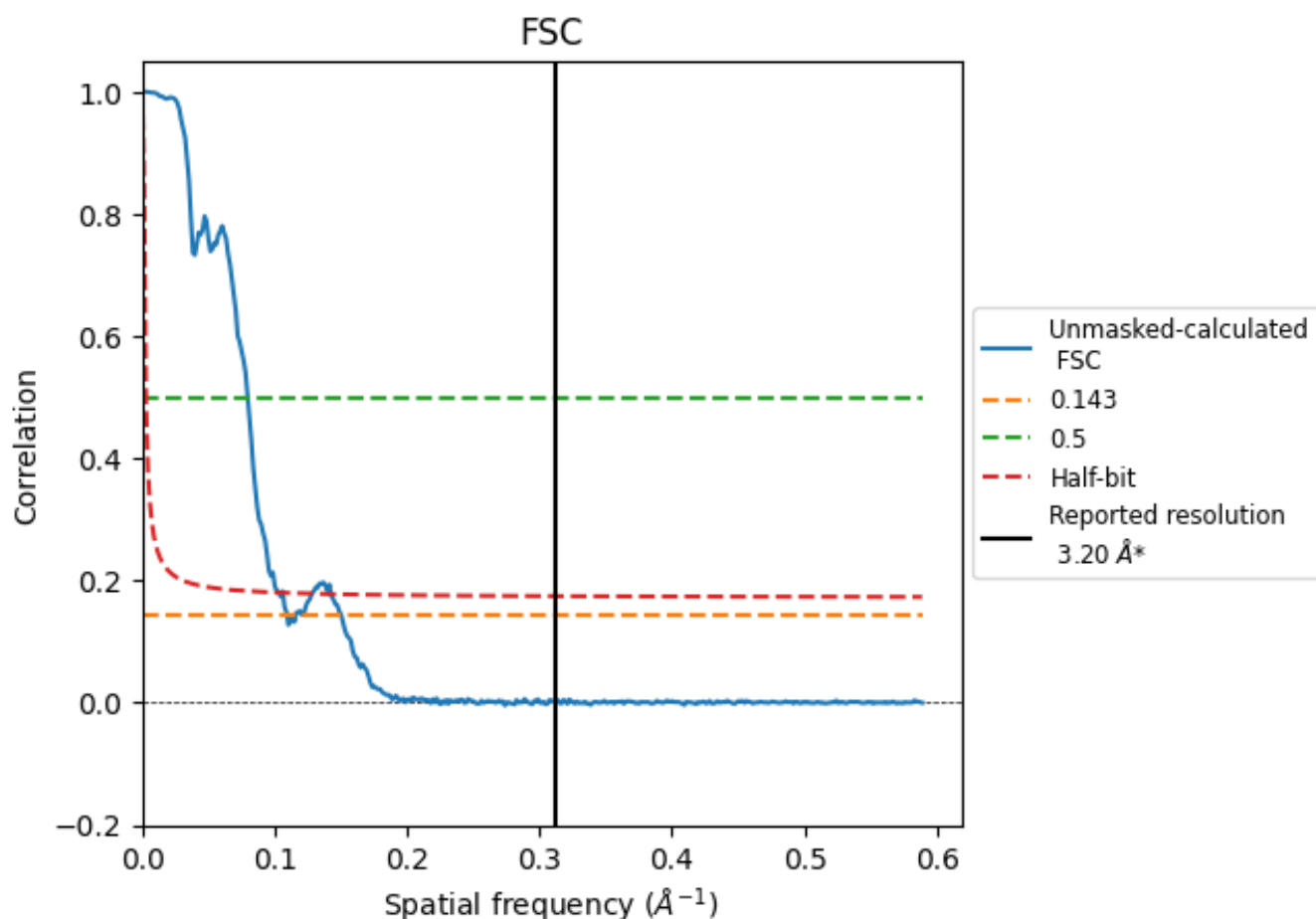


*Reported resolution corresponds to spatial frequency of 0.312 $\text{\AA}^{-1}$

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

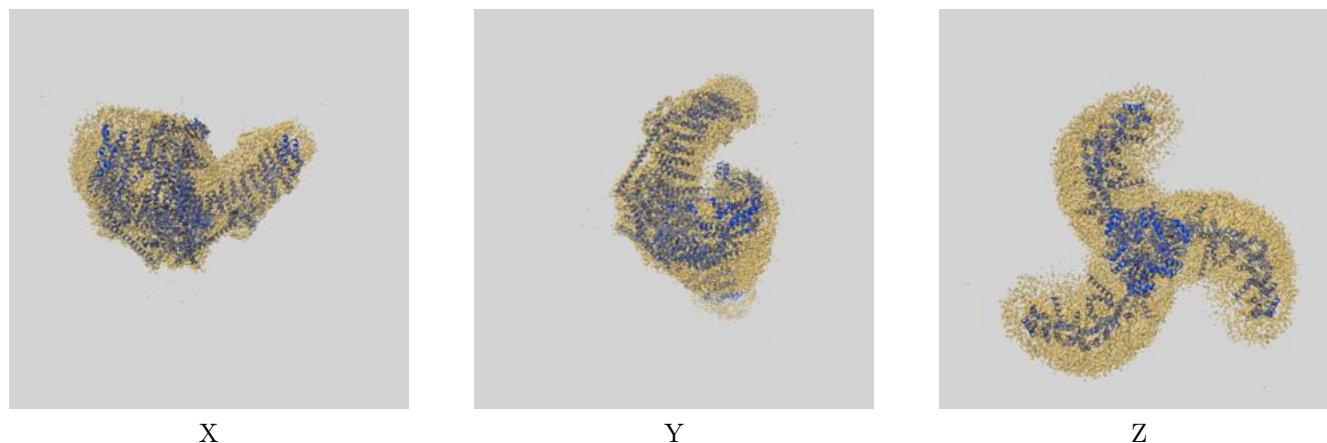
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	9.15	12.56	9.67

*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 9.15 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

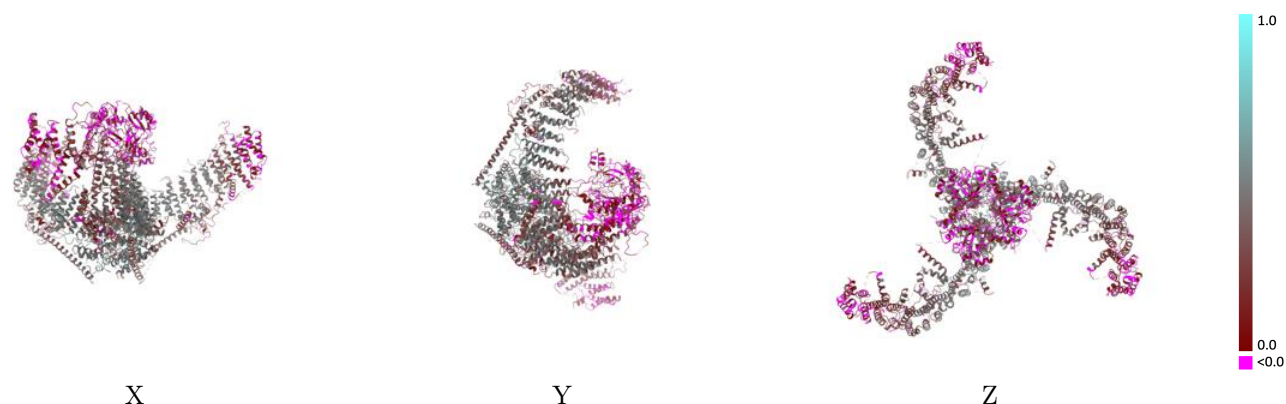
This section contains information regarding the fit between EMDB map EMD-39219 and PDB model 8YFC. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



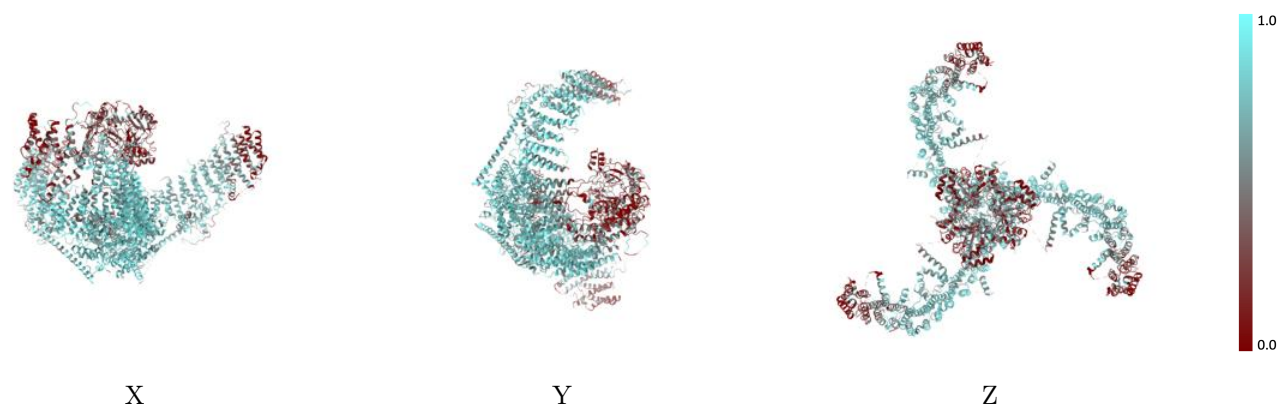
The images above show the 3D surface view of the map at the recommended contour level 0.04 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



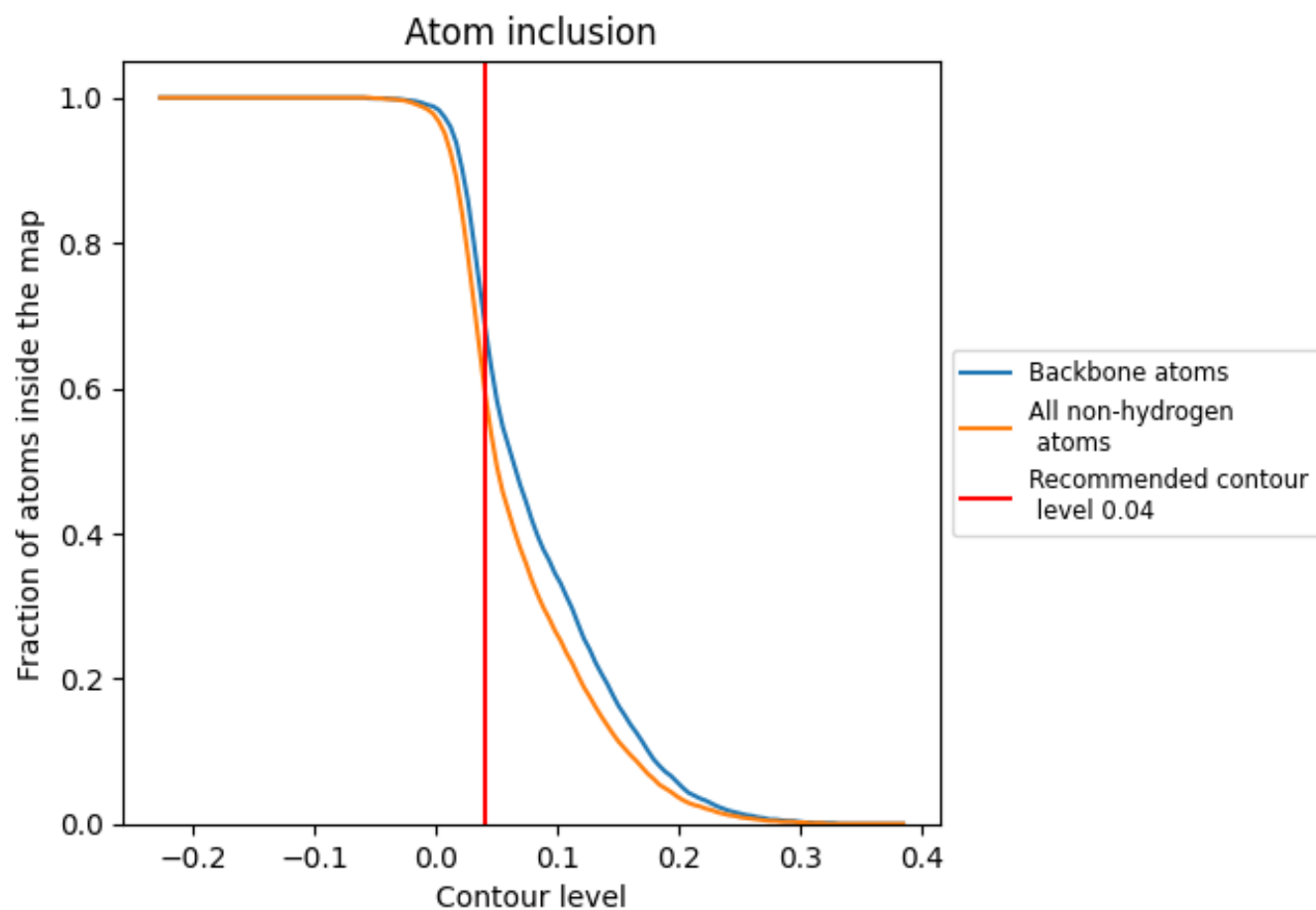
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.04).

9.4 Atom inclusion [i](#)



At the recommended contour level, 69% of all backbone atoms, 60% 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 (0.04) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6020	0.2880
A	0.6010	0.2850
B	0.6000	0.2860
C	0.6830	0.3720
D	0.6010	0.2870
E	0.6940	0.3760
F	0.6770	0.3770

1.0

0.0

<0.0