



Full wwPDB EM Validation Report ⓘ

Apr 28, 2025 – 10:40 AM EDT

PDB ID : 8VY2 / pdb_00008vy2
EMDB ID : EMD-43644
Title : Structure of mCELSR1 extracellular region containing CADH9-GAIN domains
Authors : Bandekar, S.J.; Arac, D.
Deposited on : 2024-02-06
Resolution : 4.30 Å(reported)

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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.dev118
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0rc1
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) : 2.43.1

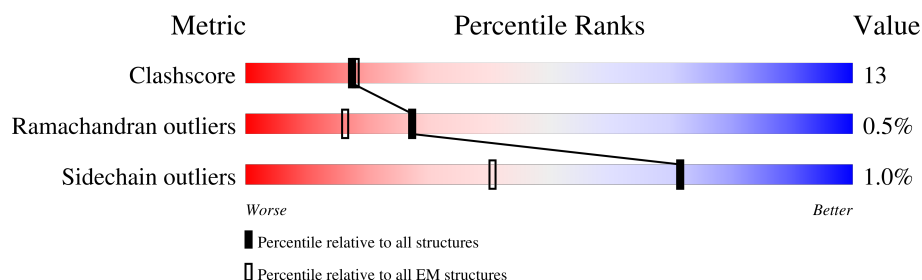
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.30 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 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	2232	
2	B	2	
2	D	2	
2	E	2	
3	C	3	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10374 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 Cadherin EGF LAG seven-pass G-type receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1319	Total	C	N	O	S	0	0
			10167	6345	1799	1934	89		

There are 9 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	254	ALA	-	expression tag	UNP O35161
A	2478	HIS	-	expression tag	UNP O35161
A	2479	HIS	-	expression tag	UNP O35161
A	2480	HIS	-	expression tag	UNP O35161
A	2481	HIS	-	expression tag	UNP O35161
A	2482	HIS	-	expression tag	UNP O35161
A	2483	HIS	-	expression tag	UNP O35161
A	2484	HIS	-	expression tag	UNP O35161
A	2485	HIS	-	expression tag	UNP O35161

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	2	Total	C	N	O	0	0
			28	16	2	10		
2	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	E	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is an oligosaccharide called beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				AltConf	Trace
3	C	3	Total	C	N	O	0	0
			39	22	2	15		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

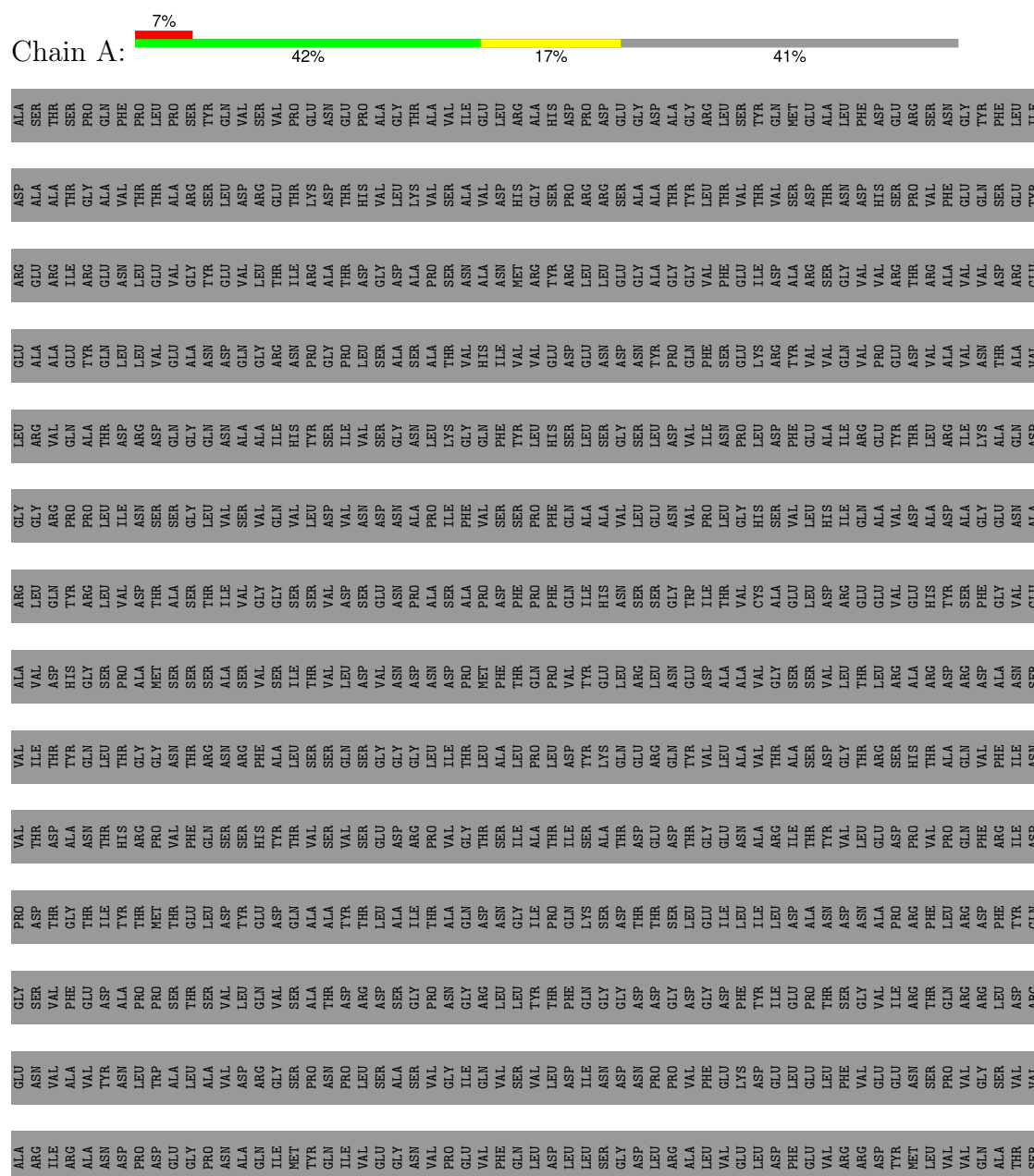


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

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: Cadherin EGF LAG seven-pass G-type receptor 1



ARG	Q2277	Y2172	E2064	P1969	V1859	W1789	V1726	S1395	L1281	N1184	ALA
ARG	V2278	R2177	V2065	W1972	R1860	H1790	W1727	R1396	P1282	R1185	PRO
ARG	V2279	R2177	L2066	W1972	M1861	H1791	W1728	W1728	P1186	L1186	LEU
R2280	R2280	H2181	Y2067	G1979	E1863	L1792	Y1729	G1399	G1283	L1187	VAL
F2281	F2281	Q2185	N2068	P1980	T1864	L1793	L1730	Y1400	G1284	L1190	SER
E2282	E2282	Q2185	N2068	P1980	T1864	I1794	G1731	T1401	T1285	M1191	ARG
D2283	D2283	Q2185	P2071	A1984	N1867	R1797	L1732	C1402	R1286	D1197	ALA
L2284	L2284	D2189	P2072	F1989	N1867	S1798	E1733	E1403	R1287	D1197	THR
Q2285	Q2285	A2073	A2073	F1989	N1867	S1798	F1734	C1404	R1288	D1197	VAL
E2286	E2286	F2074	F2074	F1989	N1867	A1799	T1736	L1609	F1289	H1200	HIS
E2287	E2287	F2074	F2074	F1989	N1867	K1800	R1737	L1614	F1290	H1200	ILE
L2288	L2288	M1994	L2078	M1994	N1873	E1801	K1738	N1429	L1295	L1206	ARG
P2289	P2289	G1998	W2079	G1998	M1873	G1802	E1739	S1629	L1295	L1206	LEU
R2289	R2289	W2080	W2080	P2081	D1875	K1803	V1742	L1436	L1306	C1206	ASP
R2290	R2290	W2081	W2081	P2081	L1877	D1804	L1743	L1437	T1307	T1207	GLN
E2291	E2291	G2086	G2086	E2004	L1877	I1805	M1744	G1643	T1307	V1210	ASN
L2292	L2292	E2215	E2215	N2005	L1877	K1806	E1745	I1438	T1308	V1210	ASP
E2293	E2293	R2103	R2103	N2005	L1877	Y1907	E1746	G1439	S1310	L1218	ASN
S2297	S2297	H2104	H2104	K2008	C1885	L1808	T1747	C1455	A1311	T1223	P1113
Y2370	Y2370	C2105	C2105	P2009	D1886	A1809	A1748	R1460	Q1312	T1223	P1114
F2299	F2299	S2106	S2106	P2010	V1867	I1810	G1749	R1460	R1313	E1227	E1115
P2299	P2299	E2219	E2219	P2010	E1888	M1811	A1652	R1460	R1314	N1228	P1117
A2300	A2300	Q2220	Q2220	A2011	D1889	M1811	A1653	Q1465	L1315	M1229	F1118
D2301	D2301	G2222	G2222	Q2012	P1890	M1811	T1750	Q1465	L1315	M1229	D1118
H2374	H2374	W2111	W2111	Q2012	P1890	M1811	S1751	T1469	D1319	K1233	F1119
D2302	D2302	L2112	L2112	D2024	W1906	M1811	R1753	F1470	M1320	F1294	Q120
R2375	R2375	S2224	S2224	D2024	W1906	M1811	L1759	R1474	N1321	L1235	F1123
P2306	P2306	E2225	E2225	S2025	Y1909	M1811	H1759	M1491	L1241	S1236	
E2307	E2307	L2116	L2116	P2021	R1903	D1818	S1761	A1492	V1243	S1236	
LVS	LVS	T2117	T2117	P2022	D1904	Q1819	H1755	A1492	Y1330	P1237	H1129
GLU	GLU	N2118	N2118	H2023	T1905	R1821	L1756	H1478	L1238	K1130	K1130
GLY	GLY	C2119	C2119	G2024	W1906	V1822	Q1757	Y1686	L1239	L1131	
PRO	PRO	F2124	F2124	S2025	Y1909	Q1823	H1758	T1480	S1240	H1132	
VAL	VAL	R2233	R2233	R2028	Y1909	I1824	L1759	P1691	L1241	S1133	
ARG	ARG	S2240	S2240	M2032	C1913	G1825	S1761	A1492	L1337	G1137	
LEU	LEU	N2241	N2241	D2032	D1914	M1826	Y1762	F1694	R1338	R1141	
THR	THR	R2244	R2244	D2034	R1915	Q1827	L1763	G1696	A1343	E1244	
ASN	ASN	N2245	N2245	G2035	G1919	P1829	F1765	K1697	T1349	A1247	
ARG	ARG	R2136	R2136	Q2036	G1919	G1830	E1766	R1499	T1252	T1252	
ARG	ARG	R2136	R2136	C2037	G1919	G1831	V1767	D1505	T1253	D1146	
THR	THR	R2140	R2140	V2043	A1925	K1831	S1768	P1704	P1447	P1147	
PRO	PRO	N2141	N2141	T2044	L1928	K1832	S1768	R1708	D1448	D148	
LEU	LEU	D2142	D2142	T2044	L1928	M1833	G1770	L1509	D1256	L1149	
THR	THR	G2143	G2143	C2048	H1933	P1771	P1771	E1510	T1262	D1151	
ALA	ALA	R2144	R2144	R2049	H1934	S1772	S1772	L1518	D1265	L1163	
GLN	GLN	R2145	R2145	R2050	V1934	I1836	W1715	L1518	T1266	D1267	
PRO	PRO	S2146	S2146	C2051	A1935	D1773	L1716	F1520	D1267	D1169	
GLU	GLU	L2147	L2147	D2052	R1939	G1839	W1717	Q1548	S1269	S1270	
PRO	PRO	R2148	R2148	D2052	R1939	G1840	A1775	Y1549	E1378	N1271	
ARG	ARG	R2148	R2148	D2052	R1939	G1840	S1776	Q1548	S1269	S1270	
ALA	ALA	L2163	L2163	A2056	S1940	V1841	M1777	Y1549	F1370	D1265	
GLU	GLU	F2164	F2164	E2057	P1941	T1778	D1721	L1518	C1375	T1266	
ARG	ARG	G2165	G2165	W2058	N1942	T1842	L1779	F1520	E1378	D1267	
THR	THR	W2166	W2166	T2059	C1951	E1843	S1780	N1554	G1391	L1273	
THR	THR	D2167	D2167	T2059	C1951	D1844	I1724	H1557	R1392	N1274	
SER	SER	V2168	V2168	G2062	E1961	V1946	R1783	L1558	C1393	V1275	
SER	SER	V2168	V2168	G2062	E1961	S1847	G1787	L1558	R1394	V1275	
ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
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ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
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ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
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ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
ARG	ARG	A2276	A2276	C2063		H1850	G1788	L1558			
ARG	ARG	A2276	A2276	C2063		H1850	G1				



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain B: 100%

NAG1
NAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D: 50%

NAG1
NAG2

- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E: 50%

NAG1
NAG2

- Molecule 3: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain C: 33% 67%

NAG1
NAG2
BMA3

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	171416	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	4.303	Depositor
Minimum map value	-2.670	Depositor
Average map value	0.004	Depositor
Map value standard deviation	0.062	Depositor
Recommended contour level	0.5	Depositor
Map size (\AA)	316.80002, 316.80002, 316.80002	wwPDB
Map dimensions	288, 288, 288	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NAG

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	0.34	0/10404	0.60	12/14138 (0.1%)

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2081	PRO	CA-C-N	-7.53	110.17	120.87
1	A	2081	PRO	C-N-CA	-7.53	110.17	120.87
1	A	1118	ASP	CA-C-N	-6.40	112.12	122.36
1	A	1118	ASP	C-N-CA	-6.40	112.12	122.36
1	A	2081	PRO	CB-CA-C	-6.06	101.56	111.56
1	A	1114	PRO	CB-CA-C	-5.73	102.10	111.56
1	A	1237	PRO	N-CA-CB	-5.56	97.41	103.25
1	A	1353	PHE	CA-CB-CG	5.30	119.10	113.80
1	A	1117	PRO	N-CA-CB	-5.12	97.88	103.25
1	A	1876	ALA	CB-CA-C	-5.08	110.31	117.23
1	A	2071	PRO	CB-CA-C	-5.07	103.19	111.56
1	A	1349	THR	N-CA-C	-5.04	107.11	114.12

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	10167	0	9781	271	0
2	B	28	0	25	0	0
2	D	28	0	25	0	0
2	E	28	0	25	1	0
3	C	39	0	34	0	0
4	A	84	0	78	0	0
All	All	10374	0	9968	271	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 13.

All (271) 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:2080:TRP:HB3	1:A:2111:TRP:CZ2	1.93	1.03
1:A:1810:VAL:HG13	1:A:1821:THR:HG22	1.62	0.81
1:A:1704:PRO:HD2	1:A:1858:GLY:HA3	1.61	0.81
1:A:1236:SER:HB3	1:A:1237:PRO:HD3	1.67	0.76
1:A:1752:SER:HA	1:A:1768:SER:O	1.86	0.75
1:A:1748:ALA:O	1:A:1752:SER:HB2	1.89	0.73
1:A:1218:LEU:HD13	1:A:1338:ARG:HA	1.71	0.72
1:A:1496:TYR:HB3	1:A:1614:LEU:HD11	1.71	0.72
1:A:1762:TYR:OH	1:A:1783:ARG:NH1	2.23	0.72
1:A:2140:ARG:HH21	1:A:2141:MET:HG2	1.55	0.72
1:A:2240:SER:OG	1:A:2244:ARG:NH1	2.24	0.70
1:A:1429:ASN:ND2	1:A:1455:CYS:O	2.26	0.69
1:A:2005:ASN:OD1	1:A:2028:ARG:NH1	2.25	0.69
1:A:1185:ARG:NH2	1:A:2249:THR:O	2.26	0.69
1:A:1989:PHE:HA	1:A:2002:CYS:HA	1.76	0.68
1:A:1281:LEU:HD12	1:A:1288:ARG:HB3	1.75	0.67
1:A:2262:ILE:HB	1:A:2358:ILE:HB	1.76	0.67
1:A:2145:ARG:NH2	1:A:2146:SER:OG	2.28	0.67
1:A:2104:HIS:HB3	1:A:2112:LEU:HD12	1.77	0.67
1:A:2281:PHE:HA	1:A:2284:ILE:HB	1.76	0.66
1:A:1183:ASN:ND2	1:A:2193:THR:O	2.28	0.66
1:A:1753:ARG:O	1:A:1767:VAL:HA	1.96	0.66
1:A:1755:HIS:O	1:A:1765:PHE:HA	1.95	0.66
1:A:1265:ASP:HB2	1:A:1274:ASN:HB2	1.77	0.65
1:A:2008:LYS:HB3	1:A:2032:MET:HE1	1.78	0.65
1:A:1915:ARG:NH2	1:A:1942:ASN:OD1	2.29	0.64
1:A:1499:ARG:HH21	1:A:1608:ASP:HB2	1.61	0.64
1:A:2452:ASN:OD1	1:A:2455:HIS:N	2.29	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1809:ALA:HB3	1:A:1822:VAL:HG12	1.78	0.64
1:A:1739:GLU:HG3	1:A:1761:SER:HB3	1.79	0.64
1:A:2447:GLU:HG3	1:A:2459:GLN:HE21	1.63	0.63
1:A:1695:GLY:O	1:A:1701:GLN:N	2.32	0.63
1:A:2185:GLN:HB2	1:A:2190:LEU:HD23	1.80	0.63
1:A:1726:VAL:HG11	1:A:1798:SER:HB3	1.80	0.62
1:A:1994:ASN:HB3	1:A:1998:GLY:H	1.63	0.62
1:A:1725:SER:H	1:A:1832:LYS:HE3	1.64	0.62
1:A:2297:SER:HB3	1:A:2410:LEU:HB2	1.81	0.62
1:A:1235:LEU:HG	1:A:1262:ILE:HD13	1.81	0.62
1:A:2253:PRO:HB3	1:A:2266:ASP:HA	1.81	0.61
1:A:2106:SER:N	1:A:2110:GLY:O	2.34	0.61
1:A:1899:HIS:HB3	1:A:1914:ASP:HB2	1.83	0.60
1:A:2355:LEU:HD11	1:A:2393:MET:HE2	1.83	0.60
1:A:2214:THR:HG1	1:A:2218:TRP:CD1	2.19	0.60
1:A:2004:GLU:OE2	1:A:2028:ARG:NH1	2.33	0.60
1:A:2214:THR:O	1:A:2218:TRP:N	2.31	0.60
1:A:1197:ASP:OD2	1:A:1200:HIS:ND1	2.34	0.60
1:A:1401:THR:HG23	1:A:1644:ARG:HE	1.67	0.60
1:A:1493:LEU:HA	1:A:1510:GLU:HG2	1.84	0.59
1:A:2109:LYS:HZ2	1:A:2112:LEU:HA	1.67	0.59
1:A:1804:ASP:HB3	1:A:1806:LYS:HZ2	1.68	0.59
1:A:1268:VAL:HG13	1:A:1269:SER:H	1.68	0.59
1:A:2362:LEU:HA	1:A:2365:LEU:HD12	1.85	0.58
1:A:1872:ASN:O	1:A:1875:ASP:N	2.34	0.58
1:A:2124:PHE:O	1:A:2128:LYS:N	2.29	0.58
1:A:1861:MET:SD	1:A:1861:MET:N	2.77	0.58
1:A:2080:TRP:CH2	1:A:2103:ARG:HB2	2.39	0.58
1:A:1334:VAL:HG21	1:A:1365:ARG:HH21	1.68	0.57
1:A:1391:GLY:HA3	1:A:1404:CYS:HA	1.87	0.57
1:A:2008:LYS:HE3	1:A:2013:ASP:HA	1.85	0.57
1:A:1754:LEU:HG	1:A:1767:VAL:HG22	1.85	0.57
1:A:1589:VAL:HG12	1:A:1919:GLY:HA3	1.86	0.57
1:A:1238:LEU:HG	1:A:1241:LEU:HD12	1.87	0.57
1:A:1748:ALA:O	1:A:1752:SER:CB	2.53	0.57
1:A:1229:MET:HG2	1:A:1233:LYS:HG3	1.87	0.56
1:A:1809:ALA:HB2	1:A:1824:ILE:HD11	1.86	0.56
1:A:1236:SER:CB	1:A:1237:PRO:HD3	2.34	0.56
1:A:1807:TYR:CD1	1:A:1829:PRO:HB3	2.40	0.56
1:A:1732:LEU:HB2	1:A:1792:LEU:HD21	1.87	0.56
1:A:2133:LYS:HA	1:A:2136:ARG:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2142:ASP:H	1:A:2145:ARG:HE	1.54	0.56
1:A:2074:PHE:HB3	1:A:2079:TRP:CH2	2.41	0.56
1:A:2109:LYS:NZ	1:A:2111:TRP:O	2.39	0.55
1:A:1227:GLU:HB2	1:A:1315:LEU:HD21	1.89	0.55
1:A:2241:ASN:OD1	1:A:2245:ASN:ND2	2.39	0.55
1:A:1900:SER:HA	1:A:1913:CYS:HA	1.89	0.55
1:A:2433:LEU:HB3	1:A:2435:THR:HG22	1.88	0.55
1:A:1370:PHE:HB3	1:A:1375:CYS:HB3	1.88	0.55
1:A:2021:PHE:CE2	1:A:2023:HIS:HB2	2.42	0.55
1:A:2279:PRO:HG2	1:A:2281:PHE:CZ	2.42	0.55
1:A:2363:GLY:HA3	1:A:2385:ILE:HG21	1.89	0.54
1:A:1496:TYR:HD2	1:A:1614:LEU:HD21	1.73	0.54
1:A:2430:ASN:HD22	1:A:2433:LEU:HG	1.73	0.54
1:A:1133:SER:HB2	1:A:1354:ARG:HH22	1.72	0.54
1:A:2172:TYR:CE2	1:A:2225:GLU:HG3	2.42	0.54
1:A:1807:TYR:C	1:A:1824:ILE:HB	2.33	0.54
1:A:1179:ARG:HH21	1:A:1182:ASP:HB2	1.72	0.54
1:A:1824:ILE:HG23	1:A:1828:LEU:CB	2.38	0.54
1:A:2420:GLU:OE2	1:A:2451:ARG:NH1	2.41	0.54
1:A:1383:TYR:CD2	1:A:1979:GLY:HA3	2.43	0.54
1:A:1793:LEU:O	1:A:1811:MET:HA	2.08	0.54
1:A:1480:THR:HG22	1:A:1548:GLN:HG2	1.89	0.53
1:A:1120:GLN:HG2	1:A:1207:THR:HB	1.90	0.53
1:A:1729:TYR:HB3	1:A:1793:LEU:HD11	1.90	0.53
1:A:1187:LEU:HD11	1:A:2250:TYR:HB2	1.91	0.53
1:A:2221:ILE:O	1:A:2224:SER:OG	2.26	0.53
1:A:1737:ARG:NH1	1:A:1786:ASP:O	2.41	0.53
1:A:1499:ARG:NH2	1:A:1505:ASP:OD2	2.42	0.53
1:A:1715:VAL:HA	1:A:1877:LEU:HD23	1.91	0.53
1:A:2226:ALA:HB1	1:A:2229:ALA:HB3	1.91	0.53
1:A:2165:GLY:HA2	1:A:2168:VAL:HG22	1.91	0.53
1:A:2275:GLY:CA	1:A:2298:PHE:O	2.57	0.53
1:A:2140:ARG:HE	1:A:2141:MET:H	1.55	0.52
1:A:2124:PHE:HA	1:A:2127:LEU:HB2	1.91	0.52
1:A:1757:GLN:CD	1:A:1759:LEU:HB2	2.35	0.52
1:A:2430:ASN:OD1	1:A:2431:HIS:N	2.43	0.52
1:A:1392:ARG:HH12	1:A:1394:ARG:HG2	1.74	0.52
1:A:1746:ALA:HB3	1:A:1754:LEU:HB2	1.92	0.51
1:A:1163:LEU:HD11	1:A:2248:ARG:HB3	1.91	0.51
1:A:1119:PHE:O	1:A:1206:CYS:HA	2.11	0.51
1:A:1319:ASP:OD1	1:A:1320:ASN:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1903:ARG:HD3	1:A:1912:ILE:HG13	1.93	0.51
1:A:2037:CYS:HB2	1:A:2048:CYS:SG	2.51	0.51
1:A:2059:THR:OG1	1:A:2064:GLU:OE1	2.21	0.51
1:A:1191:MET:HB2	1:A:1206:CYS:SG	2.51	0.51
1:A:2218:TRP:HA	1:A:2221:ILE:HD12	1.92	0.51
1:A:1470:PHE:HE1	1:A:1651:PHE:HB3	1.75	0.50
1:A:1824:ILE:HG23	1:A:1828:LEU:HB3	1.93	0.50
1:A:2203:VAL:HG11	1:A:2256:ILE:HG21	1.93	0.50
1:A:1392:ARG:NH1	1:A:1394:ARG:HG2	2.26	0.50
1:A:2141:MET:HE1	1:A:2177:ARG:HB3	1.92	0.50
1:A:1843:GLU:OE1	1:A:1849:ARG:NH2	2.45	0.50
1:A:2056:ALA:HA	1:A:2065:VAL:HA	1.92	0.50
1:A:1290:PHE:HB3	1:A:1295:LEU:HG	1.93	0.50
1:A:1478:HIS:HA	1:A:1549:TYR:O	2.11	0.50
1:A:1842:THR:HA	1:A:1849:ARG:HH21	1.76	0.50
1:A:2380:PRO:HG2	1:A:2383:PRO:HB3	1.93	0.50
1:A:2275:GLY:HA3	1:A:2298:PHE:O	2.12	0.50
1:A:1197:ASP:OD1	1:A:1200:HIS:N	2.27	0.49
1:A:1396:ARG:HG2	1:A:1399:GLY:C	2.37	0.49
1:A:2419:GLU:OE1	1:A:2421:ARG:NE	2.46	0.49
1:A:1753:ARG:HH21	1:A:1755:HIS:CE1	2.30	0.49
1:A:2034:THR:HG23	1:A:2036:GLN:H	1.78	0.49
1:A:1244:GLU:HB2	1:A:1254:LYS:HE2	1.94	0.49
1:A:2430:ASN:HB3	1:A:2433:LEU:HB2	1.95	0.49
1:A:1337:LEU:HD23	1:A:1360:THR:HA	1.95	0.49
1:A:1859:VAL:HG13	1:A:1861:MET:HE1	1.94	0.49
1:A:1508:ALA:O	1:A:1518:LEU:HD12	2.13	0.49
1:A:2080:TRP:HB3	1:A:2111:TRP:CE2	2.44	0.49
1:A:1190:LEU:O	1:A:1191:MET:HE2	2.13	0.48
1:A:2424:PRO:HB3	1:A:2470:MET:SD	2.53	0.48
1:A:1915:ARG:O	1:A:1939:ARG:NH2	2.46	0.48
1:A:1343:ALA:HB3	1:A:1355:PRO:HG2	1.95	0.48
1:A:2233:ARG:NH2	1:A:2431:HIS:O	2.46	0.48
1:A:1469:THR:HB	1:A:1653:ALA:HB3	1.94	0.48
1:A:2277:GLN:HG3	1:A:2280:ARG:NH1	2.29	0.48
1:A:1306:LEU:O	1:A:1310:SER:OG	2.32	0.48
1:A:1804:ASP:HB3	1:A:1806:LYS:NZ	2.28	0.48
1:A:1933:HIS:CE1	1:A:1961:GLU:HA	2.49	0.48
1:A:2141:MET:HB2	1:A:2145:ARG:NH2	2.28	0.48
1:A:2277:GLN:HG3	1:A:2280:ARG:HH11	1.79	0.48
1:A:1716:LEU:HG	1:A:1837:VAL:HG22	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1825:GLY:O	1:A:1827:GLN:N	2.47	0.47
1:A:1474:ARG:NH2	1:A:1609:LEU:O	2.43	0.47
1:A:1585:PHE:CE2	1:A:1928:LEU:HD23	2.50	0.47
1:A:1742:VAL:HG22	1:A:1755:HIS:CE1	2.49	0.47
1:A:1391:GLY:CA	1:A:1404:CYS:HA	2.44	0.47
1:A:1507:ILE:HG22	1:A:1520:PHE:HB2	1.96	0.47
1:A:2429:TRP:CD2	1:A:2440:GLY:HA2	2.50	0.47
1:A:1234:PHE:HB3	1:A:1262:ILE:HD11	1.95	0.47
1:A:1695:GLY:O	1:A:1700:GLU:N	2.48	0.47
1:A:1724:ILE:HG22	1:A:1832:LYS:HB2	1.97	0.47
1:A:2225:GLU:HG2	1:A:2227:GLY:N	2.30	0.47
1:A:1307:THR:HG23	1:A:1312:GLN:O	2.15	0.47
1:A:1735:ARG:NE	1:A:1787:GLY:O	2.45	0.47
1:A:2004:GLU:O	1:A:2005:ASN:HB2	2.15	0.46
1:A:1141:ARG:CZ	1:A:1172:THR:HB	2.45	0.46
1:A:1306:LEU:HA	1:A:1309:ILE:HG22	1.97	0.46
1:A:1685:THR:OG1	1:A:1686:TYR:N	2.48	0.46
1:A:1691:PRO:HG2	1:A:1694:PHE:HD2	1.80	0.46
1:A:2078:ILE:C	1:A:2080:TRP:H	2.24	0.46
1:A:2079:TRP:O	1:A:2080:TRP:C	2.58	0.46
1:A:2080:TRP:CE2	1:A:2103:ARG:HD2	2.50	0.46
1:A:2145:ARG:HA	1:A:2148:ARG:HG2	1.98	0.46
1:A:1554:ASN:ND2	1:A:1564:PRO:O	2.49	0.46
1:A:1708:ARG:NH2	1:A:1887:VAL:HG13	2.31	0.46
1:A:1720:LEU:HD21	1:A:1834:ARG:O	2.16	0.46
1:A:1394:ARG:HH22	1:A:1642:ASP:C	2.24	0.46
1:A:1826:ASN:C	1:A:1829:PRO:HD2	2.41	0.46
1:A:2270:LYS:HD2	1:A:2349:GLY:O	2.15	0.45
1:A:1266:THR:O	1:A:1267:ASP:C	2.59	0.45
1:A:1969:PRO:HG2	1:A:1972:TRP:CD1	2.51	0.45
1:A:2142:ASP:O	1:A:2145:ARG:NH2	2.49	0.45
1:A:2057:GLU:OE1	1:A:2071:PRO:HB3	2.16	0.45
1:A:1764:ARG:NE	1:A:1766:GLU:OE2	2.49	0.45
1:A:2361:THR:O	1:A:2365:LEU:HG	2.16	0.45
1:A:1675:ASN:OD1	1:A:1675:ASN:N	2.49	0.45
1:A:1749:GLY:HA2	1:A:1834:ARG:CZ	2.47	0.45
1:A:1769:TYR:CD1	1:A:1831:LEU:HD13	2.52	0.45
1:A:1268:VAL:HG13	1:A:1269:SER:N	2.31	0.45
1:A:1713:SER:HA	1:A:1880:ARG:HB3	1.97	0.45
1:A:1824:ILE:HG22	1:A:1829:PRO:HG3	1.99	0.45
1:A:1737:ARG:HH21	1:A:1906:TRP:HB3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1729:TYR:CD2	1:A:1864:THR:HA	2.52	0.44
1:A:2008:LYS:HB2	1:A:2015:CYS:HB3	1.99	0.44
1:A:2212:PRO:O	1:A:2215:GLU:HG2	2.18	0.44
1:A:1284:GLY:O	1:A:1286:ARG:NH1	2.50	0.44
1:A:1118:ASP:OD2	1:A:1205:LEU:HB2	2.17	0.44
1:A:1465:GLN:HB3	2:E:1:NAG:H61	1.99	0.44
1:A:2142:ASP:O	1:A:2146:SER:OG	2.30	0.44
1:A:1733:MET:CE	1:A:1789:TRP:HB3	2.48	0.44
1:A:2298:PHE:HD2	1:A:2302:THR:HG21	1.82	0.44
1:A:2288:LEU:HD23	1:A:2293:GLU:HG2	2.00	0.44
1:A:1720:LEU:HD23	1:A:1720:LEU:H	1.83	0.43
1:A:1737:ARG:NH2	1:A:1905:THR:O	2.51	0.43
1:A:1864:THR:N	1:A:1867:ASN:OD1	2.50	0.43
1:A:2032:MET:O	1:A:2034:THR:N	2.52	0.43
1:A:2431:HIS:HA	1:A:2438:THR:O	2.19	0.43
1:A:1239:LEU:HD23	1:A:1239:LEU:H	1.84	0.43
1:A:2071:PRO:HB2	1:A:2072:ARG:H	1.45	0.43
1:A:1776:SER:OG	1:A:1778:GLN:OE1	2.37	0.43
1:A:1242:PHE:C	1:A:1244:GLU:N	2.77	0.43
1:A:1717:TRP:HB2	1:A:1836:ILE:CG2	2.48	0.43
1:A:1810:VAL:HG22	1:A:1821:THR:HB	2.01	0.43
1:A:1969:PRO:HG2	1:A:1972:TRP:CG	2.54	0.43
1:A:1764:ARG:HG3	1:A:1778:GLN:OE1	2.19	0.43
1:A:2127:LEU:HD23	1:A:2127:LEU:HA	1.82	0.43
1:A:1769:TYR:H	1:A:1774:VAL:HG23	1.84	0.43
1:A:2103:ARG:HD3	1:A:2111:TRP:HB3	2.01	0.43
1:A:1123:PHE:HB3	1:A:1210:VAL:HG22	2.01	0.42
1:A:1312:GLN:HE21	1:A:1314:VAL:HB	1.84	0.42
1:A:2277:GLN:HE22	1:A:2281:PHE:N	2.17	0.42
1:A:1141:ARG:HG2	1:A:1174:GLU:HA	2.01	0.42
1:A:1762:TYR:CD1	1:A:1780:SER:HA	2.55	0.42
1:A:1809:ALA:HB3	1:A:1822:VAL:CG1	2.48	0.42
1:A:1824:ILE:HG23	1:A:1828:LEU:HB2	2.00	0.42
1:A:2141:MET:HA	1:A:2145:ARG:HE	1.84	0.42
1:A:1228:ASN:N	1:A:1271:ASN:O	2.51	0.42
1:A:1436:LEU:HB2	1:A:1439:GLY:O	2.20	0.42
1:A:1589:VAL:CG1	1:A:1919:GLY:HA3	2.49	0.42
1:A:1733:MET:SD	1:A:1791:HIS:HB2	2.59	0.42
1:A:2220:GLN:O	1:A:2223:ARG:HG2	2.20	0.42
1:A:1235:LEU:HD23	1:A:1235:LEU:HA	1.72	0.42
1:A:1499:ARG:NH2	1:A:1608:ASP:HB2	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1825:GLY:O	1:A:1828:LEU:N	2.46	0.42
1:A:1117:PRO:O	1:A:1118:ASP:C	2.63	0.42
1:A:1729:TYR:HA	1:A:1794:ILE:O	2.20	0.42
1:A:1818:ASP:OD1	1:A:1819:GLN:N	2.53	0.42
1:A:1273:LEU:HD12	1:A:1273:LEU:HA	1.86	0.42
1:A:2074:PHE:CD1	1:A:2074:PHE:N	2.87	0.42
1:A:1402:CYS:C	1:A:1404:CYS:H	2.28	0.41
1:A:1585:PHE:HD2	1:A:1589:VAL:HG23	1.85	0.41
1:A:2280:ARG:HB3	1:A:2283:ASP:HB3	2.02	0.41
1:A:2425:VAL:HG12	1:A:2427:VAL:HG13	2.01	0.41
1:A:1722:ILE:HD13	1:A:1728:TRP:CZ2	2.55	0.41
1:A:1756:LEU:HA	1:A:1764:ARG:O	2.20	0.41
1:A:2141:MET:SD	1:A:2181:HIS:HB2	2.60	0.41
1:A:1757:GLN:HG3	1:A:1759:LEU:H	1.86	0.41
1:A:1984:ALA:O	1:A:1989:PHE:HB2	2.20	0.41
1:A:2274:THR:C	1:A:2300:ALA:HA	2.45	0.41
1:A:1330:TYR:CE2	1:A:1563:GLY:HA2	2.55	0.41
1:A:1934:VAL:HG12	1:A:1934:VAL:O	2.20	0.41
1:A:1804:ASP:OD1	1:A:1805:ILE:N	2.52	0.41
1:A:1242:PHE:O	1:A:1244:GLU:N	2.54	0.41
1:A:1730:LEU:HB2	1:A:1794:ILE:HB	2.02	0.41
1:A:2008:LYS:HA	1:A:2015:CYS:HA	2.03	0.41
1:A:2270:LYS:NZ	1:A:2397:GLU:O	2.54	0.41
1:A:1370:PHE:CE2	1:A:1378:GLU:HG2	2.55	0.41
1:A:1460:ARG:HD2	1:A:1648:MET:HB3	2.02	0.41
1:A:1491:ASN:OD1	1:A:1629:SER:OG	2.38	0.41
1:A:1383:TYR:CZ	1:A:1980:PRO:HD2	2.55	0.41
1:A:1807:TYR:O	1:A:1824:ILE:HB	2.21	0.41
1:A:2044:ILE:HG12	1:A:2050:ARG:O	2.21	0.41
1:A:2086:GLY:C	1:A:2104:HIS:HE1	2.29	0.41
1:A:1841:VAL:HB	1:A:1850:HIS:HD2	1.86	0.40
1:A:1890:PRO:HB2	1:A:1909:TYR:HD2	1.85	0.40
1:A:1247:ALA:HB1	1:A:1252:THR:O	2.20	0.40
1:A:1735:ARG:HD2	1:A:1789:TRP:CE2	2.56	0.40
1:A:1234:PHE:HD1	1:A:1234:PHE:HA	1.76	0.40
1:A:1697:LYS:HD2	1:A:1697:LYS:HA	1.88	0.40
1:A:1872:ASN:O	1:A:1873:MET:C	2.65	0.40
1:A:2430:ASN:O	1:A:2439:GLY:HA3	2.22	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	1315/2232 (59%)	1209 (92%)	100 (8%)	6 (0%)	25 63

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1236	SER
1	A	1237	PRO
1	A	2071	PRO
1	A	1114	PRO
1	A	1697	LYS
1	A	1117	PRO

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	1135/1915 (59%)	1124 (99%)	11 (1%)	73 82

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1116	LEU
1	A	1223	THR
1	A	1229	MET
1	A	1234	PHE
1	A	1238	LEU

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Mol	Chain	Res	Type
1	A	1275	VAL
1	A	1835	THR
1	A	2072	ARG
1	A	2115	GLU
1	A	2119	CYS
1	A	2133	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1120	GLN
1	A	1261	ASN
1	A	1329	ASN
1	A	1390	ASN
1	A	1412	HIS
1	A	1442	HIS
1	A	1475	GLN
1	A	1501	ASN
1	A	1554	ASN
1	A	1557	HIS
1	A	1674	GLN
1	A	1778	GLN
1	A	1826	ASN
1	A	1850	HIS
1	A	1899	HIS
1	A	1933	HIS
1	A	2012	GLN
1	A	2100	ASN
1	A	2104	HIS
1	A	2118	ASN
1	A	2131	ASN
1	A	2135	ASN
1	A	2199	HIS
1	A	2204	HIS
1	A	2222	GLN
1	A	2234	HIS
1	A	2272	ASN
1	A	2459	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 ⓘ

9 monosaccharides 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	NAG	B	1	2,1	14,14,15	0.34	0	17,19,21	0.83	0
2	NAG	B	2	2	14,14,15	0.30	0	17,19,21	0.68	0
3	NAG	C	1	3,1	14,14,15	0.31	0	17,19,21	0.99	1 (5%)
3	NAG	C	2	3	14,14,15	0.27	0	17,19,21	1.05	2 (11%)
3	BMA	C	3	3	11,11,12	0.24	0	15,15,17	0.54	0
2	NAG	D	1	2,1	14,14,15	0.27	0	17,19,21	1.14	2 (11%)
2	NAG	D	2	2	14,14,15	0.28	0	17,19,21	0.73	0
2	NAG	E	1	2,1	14,14,15	0.28	0	17,19,21	1.08	2 (11%)
2	NAG	E	2	2	14,14,15	0.29	0	17,19,21	0.97	1 (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	NAG	B	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	B	2	2	-	2/6/23/26	0/1/1/1
3	NAG	C	1	3,1	-	3/6/23/26	0/1/1/1
3	NAG	C	2	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BMA	C	3	3	-	0/2/19/22	0/1/1/1
2	NAG	D	1	2,1	-	5/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	2,1	-	3/6/23/26	0/1/1/1
2	NAG	E	2	2	-	3/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1	NAG	C2-N2-C7	3.56	127.67	122.90
3	C	1	NAG	C1-O5-C5	3.12	116.37	112.19
2	D	1	NAG	C2-N2-C7	3.11	127.07	122.90
2	E	2	NAG	C1-O5-C5	2.71	115.82	112.19
3	C	2	NAG	C1-O5-C5	2.49	115.53	112.19
3	C	2	NAG	C2-N2-C7	2.20	125.85	122.90
2	E	1	NAG	C1-C2-N2	-2.10	107.13	110.43
2	D	1	NAG	C1-O5-C5	2.01	114.88	112.19

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C1-C2-N2-C7
2	D	2	NAG	C8-C7-N2-C2
2	D	2	NAG	O7-C7-N2-C2
2	E	1	NAG	C3-C2-N2-C7
2	E	1	NAG	C8-C7-N2-C2
2	E	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C3-C2-N2-C7
2	E	2	NAG	O7-C7-N2-C2
3	C	1	NAG	C1-C2-N2-C7
3	C	1	NAG	C8-C7-N2-C2
3	C	1	NAG	O7-C7-N2-C2
2	E	2	NAG	C8-C7-N2-C2
2	B	1	NAG	C8-C7-N2-C2
2	B	1	NAG	O7-C7-N2-C2
3	C	2	NAG	C8-C7-N2-C2
3	C	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C8-C7-N2-C2

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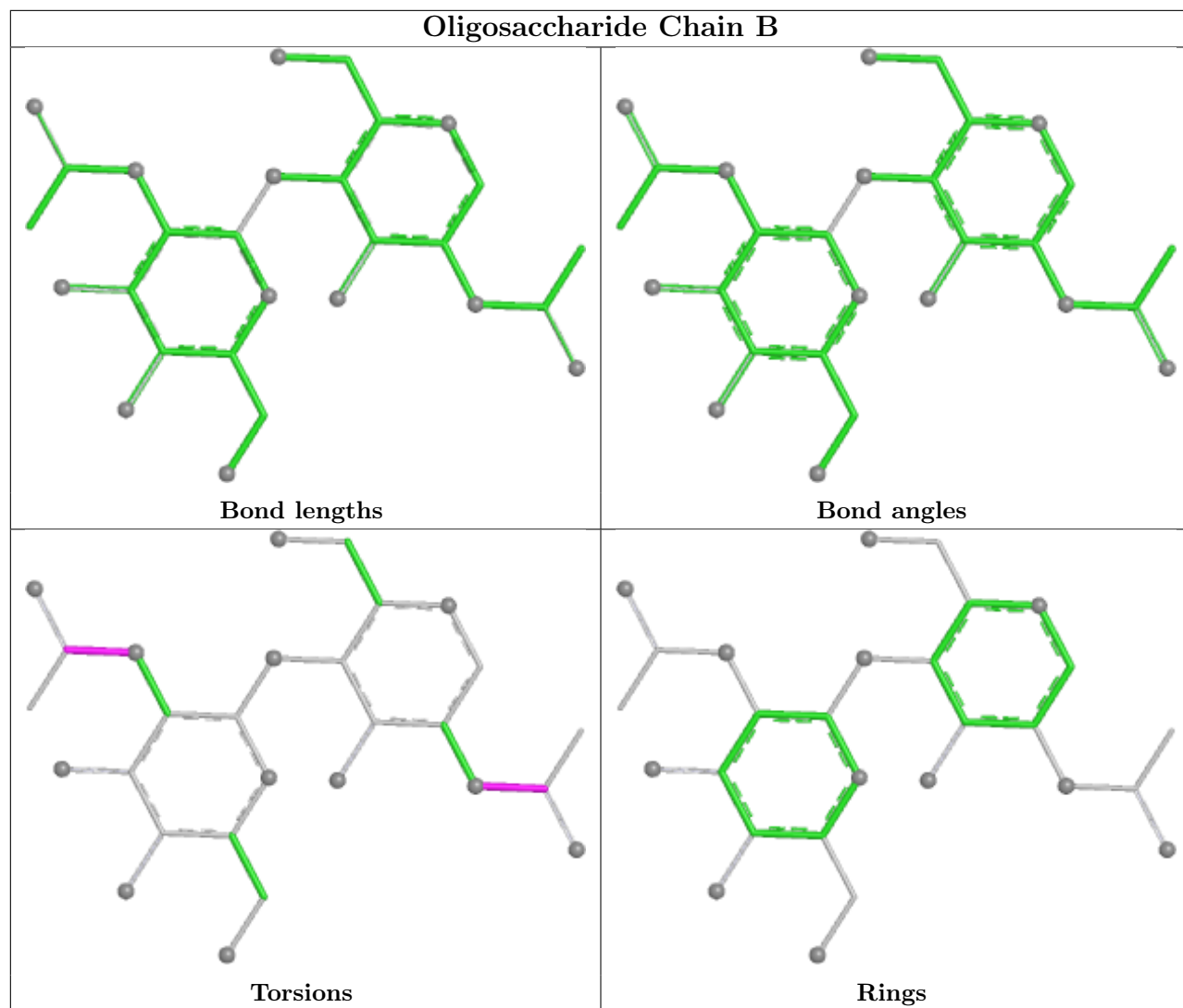
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	O7-C7-N2-C2
2	D	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7
2	B	2	NAG	C8-C7-N2-C2
2	B	2	NAG	O7-C7-N2-C2
2	D	1	NAG	C4-C5-C6-O6

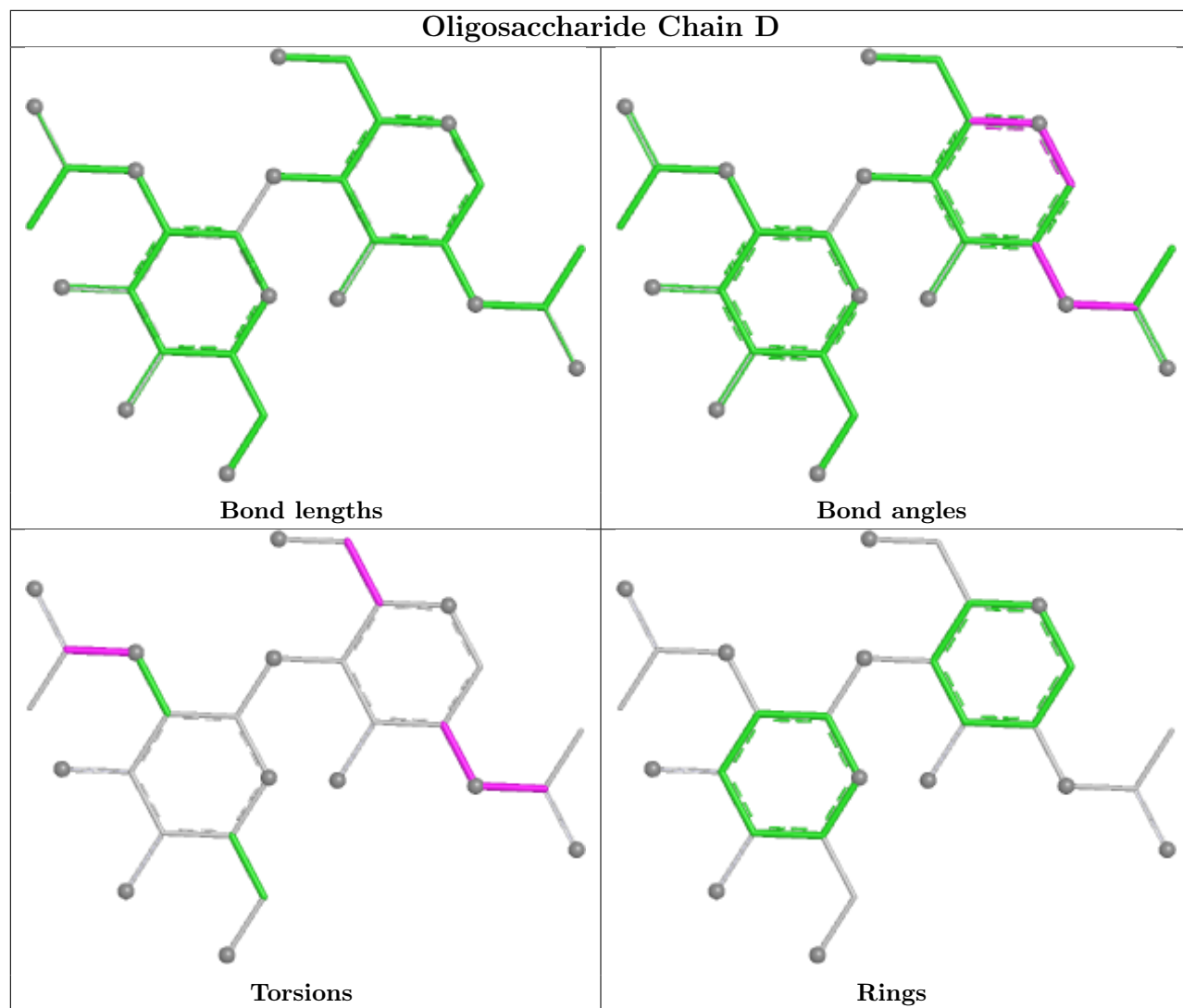
There are no ring outliers.

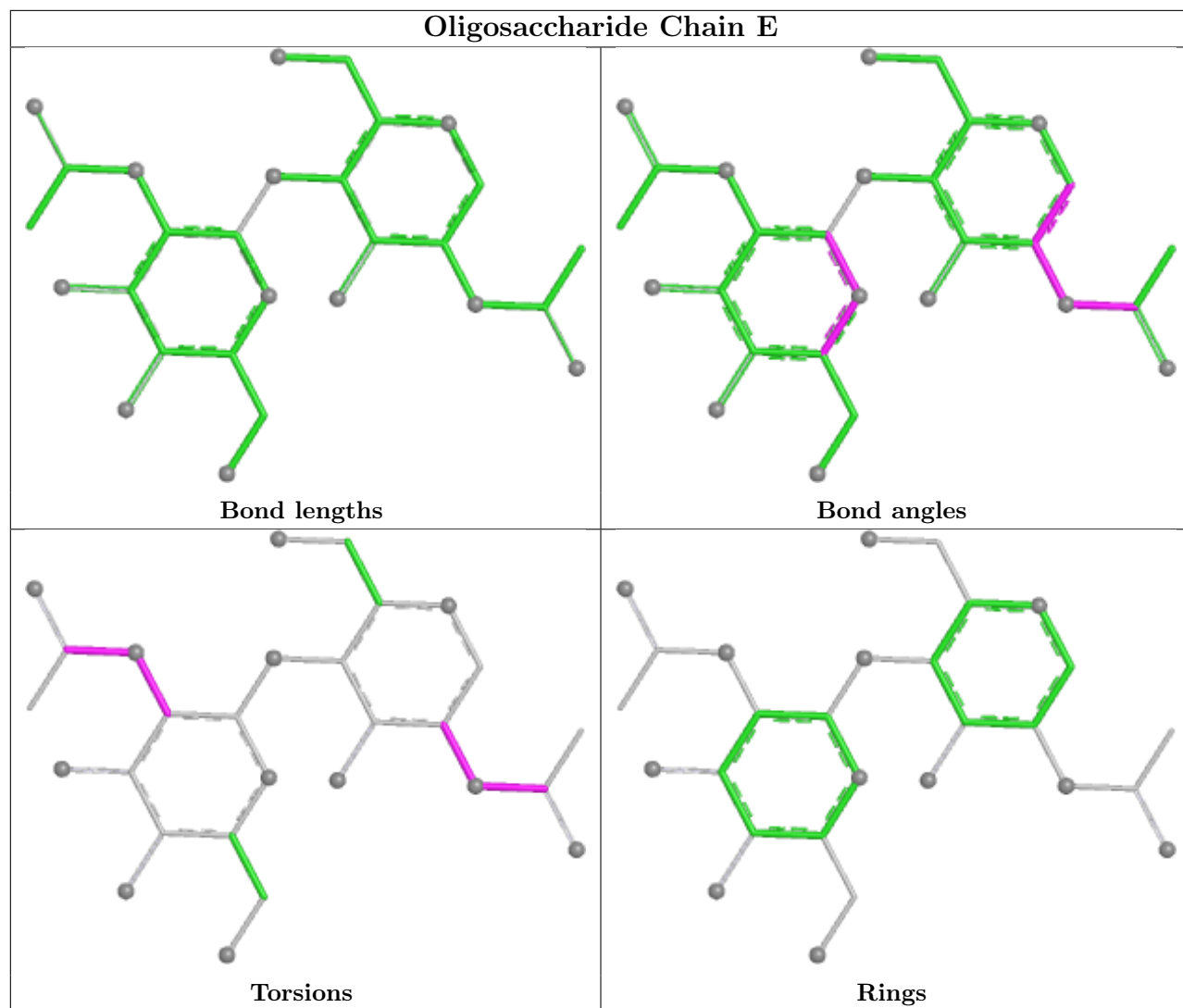
1 monomer is involved in 1 short contact:

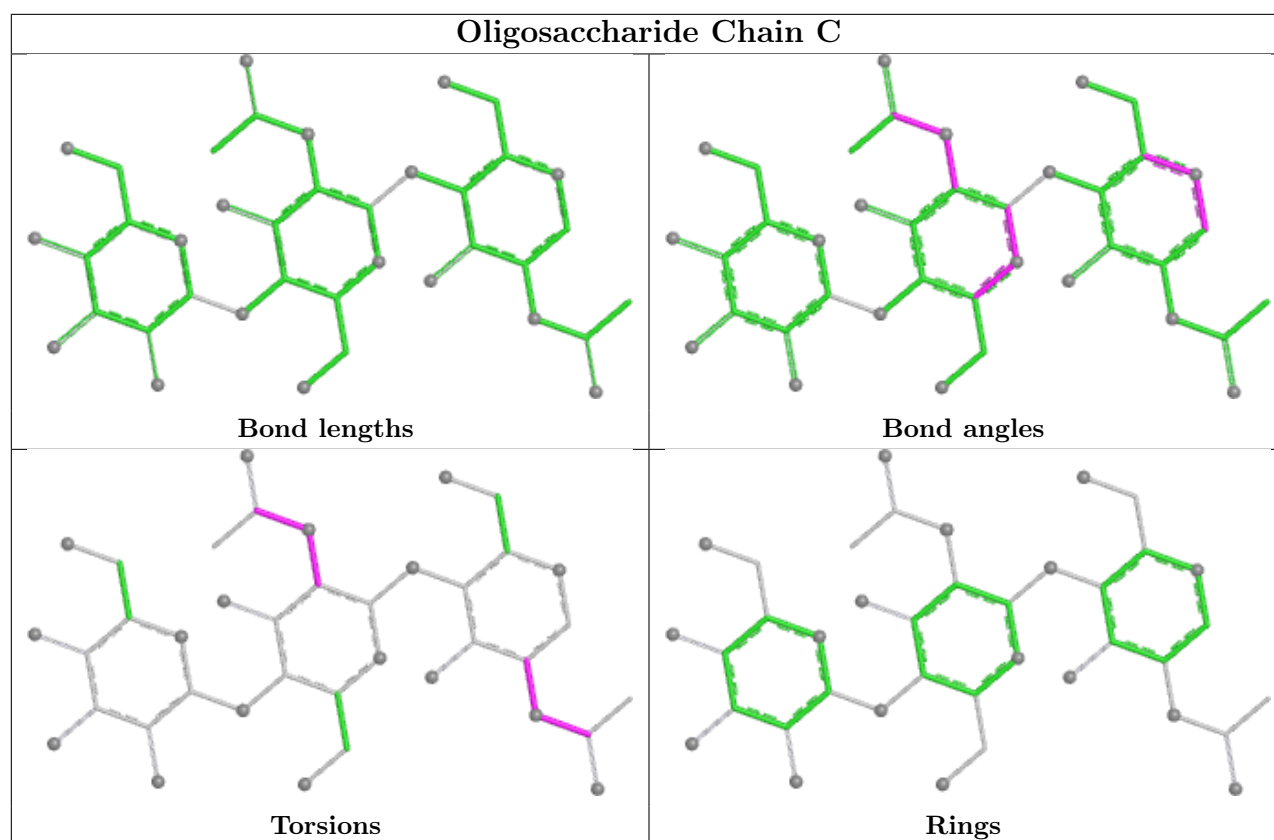
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

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	$\# Z > 2$
4	NAG	A	2503	1	14,14,15	0.28	0	17,19,21	0.55	0
4	NAG	A	2505	1	14,14,15	0.26	0	17,19,21	0.58	0
4	NAG	A	2506	1	14,14,15	0.28	0	17,19,21	0.54	0
4	NAG	A	2504	1	14,14,15	0.30	0	17,19,21	0.62	0
4	NAG	A	2501	1	14,14,15	0.28	0	17,19,21	0.52	0
4	NAG	A	2502	1	14,14,15	0.32	0	17,19,21	0.66	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
4	NAG	A	2503	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2505	1	-	4/6/23/26	0/1/1/1
4	NAG	A	2506	1	-	3/6/23/26	0/1/1/1
4	NAG	A	2504	1	-	3/6/23/26	0/1/1/1
4	NAG	A	2501	1	-	3/6/23/26	0/1/1/1
4	NAG	A	2502	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2501	NAG	C8-C7-N2-C2
4	A	2501	NAG	O7-C7-N2-C2
4	A	2502	NAG	C8-C7-N2-C2
4	A	2502	NAG	O7-C7-N2-C2
4	A	2503	NAG	C8-C7-N2-C2
4	A	2503	NAG	O7-C7-N2-C2
4	A	2505	NAG	C8-C7-N2-C2
4	A	2505	NAG	O7-C7-N2-C2
4	A	2505	NAG	O5-C5-C6-O6
4	A	2501	NAG	O5-C5-C6-O6
4	A	2506	NAG	O5-C5-C6-O6
4	A	2506	NAG	C8-C7-N2-C2
4	A	2504	NAG	C1-C2-N2-C7
4	A	2505	NAG	C1-C2-N2-C7
4	A	2504	NAG	C8-C7-N2-C2
4	A	2506	NAG	O7-C7-N2-C2
4	A	2504	NAG	O7-C7-N2-C2

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

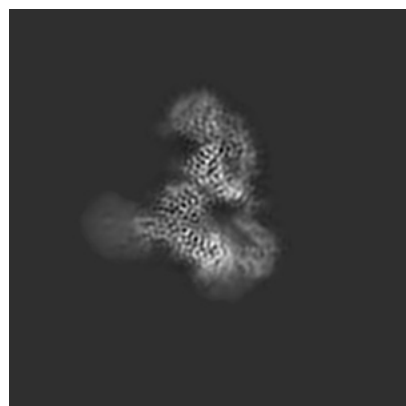
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-43644. These allow visual inspection of the internal detail of the map and identification of artifacts.

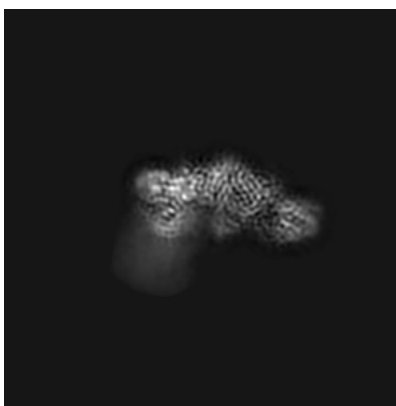
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

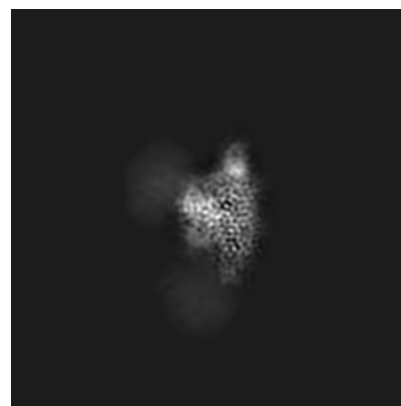
6.1.1 Primary map



X

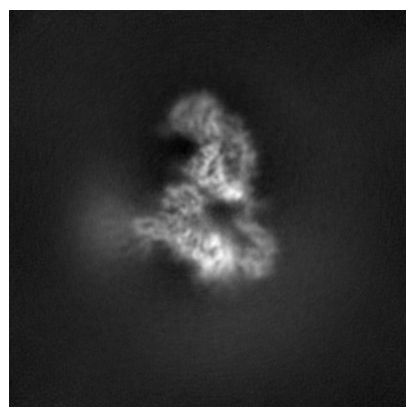


Y

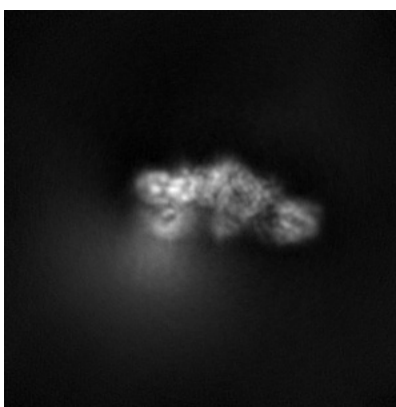


Z

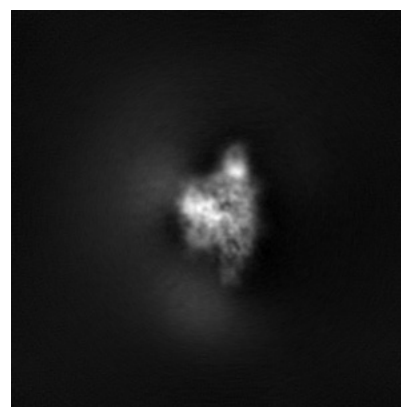
6.1.2 Raw map



X



Y

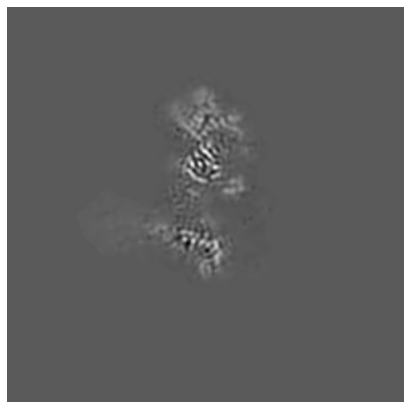


Z

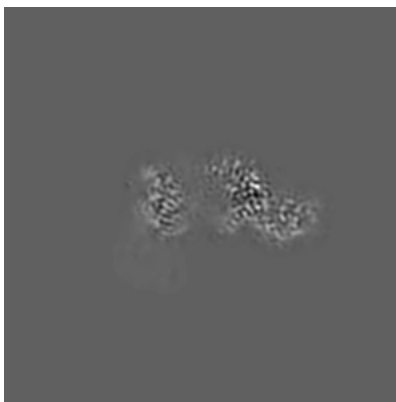
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 144

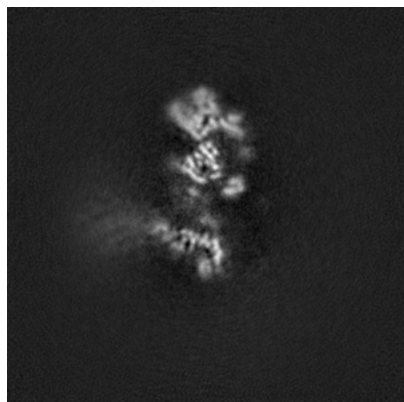


Y Index: 144

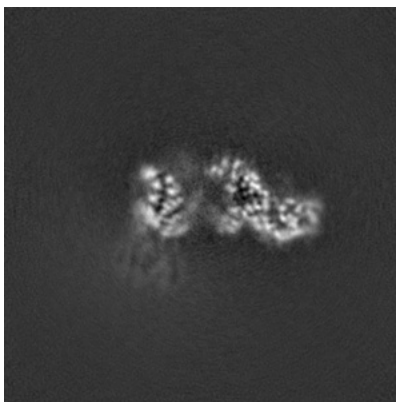


Z Index: 144

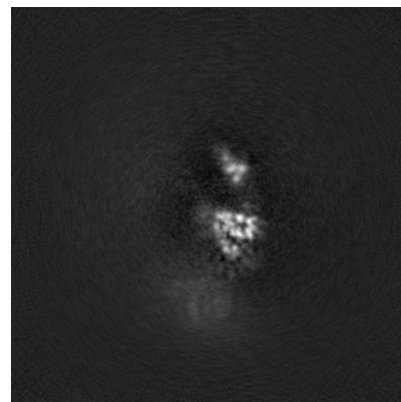
6.2.2 Raw map



X Index: 144



Y Index: 144

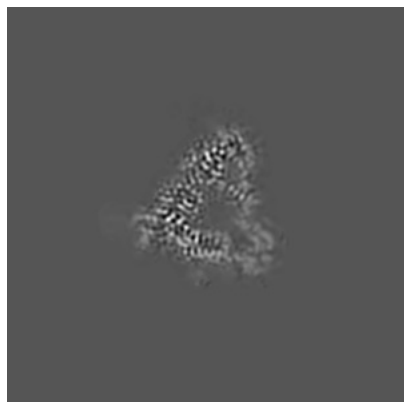


Z Index: 144

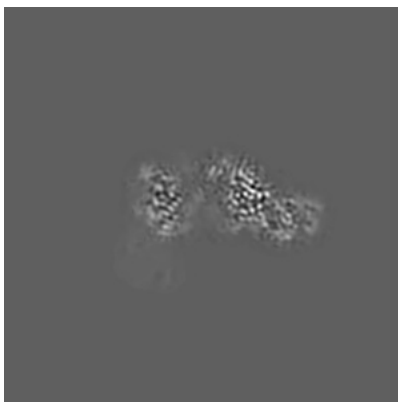
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

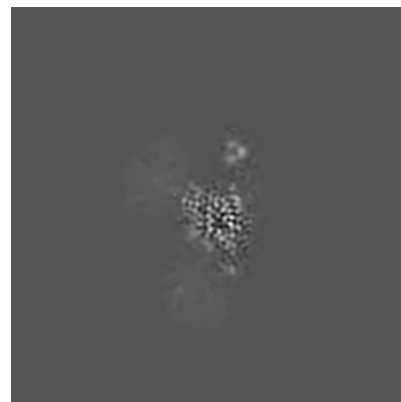
6.3.1 Primary map



X Index: 159

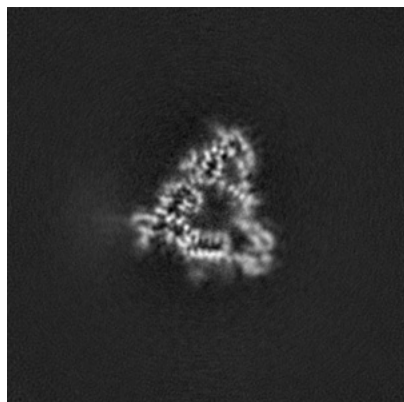


Y Index: 142

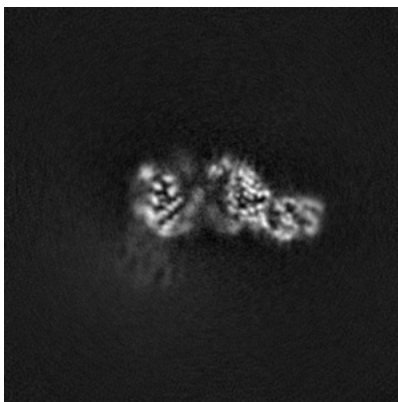


Z Index: 120

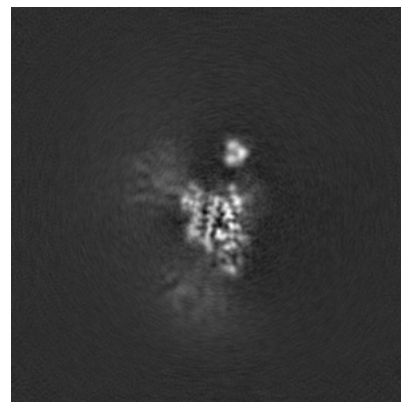
6.3.2 Raw map



X Index: 159



Y Index: 142

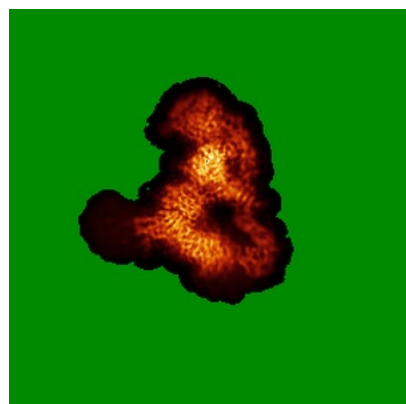


Z Index: 121

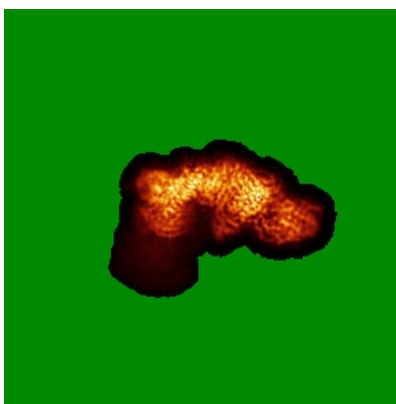
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) ⓘ

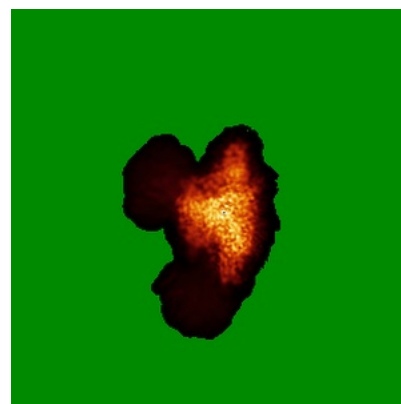
6.4.1 Primary map



X

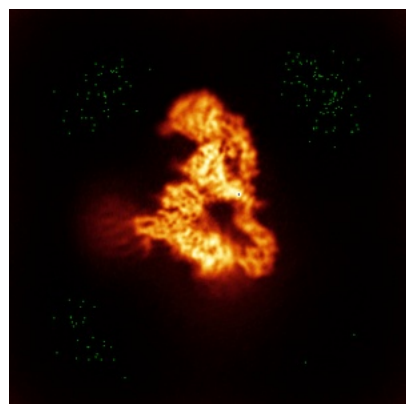


Y

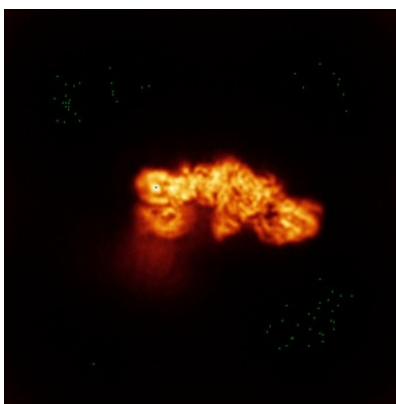


Z

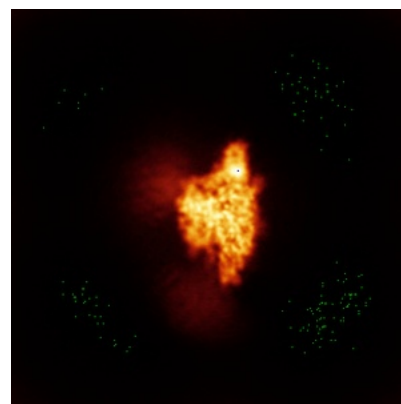
6.4.2 Raw map



X



Y

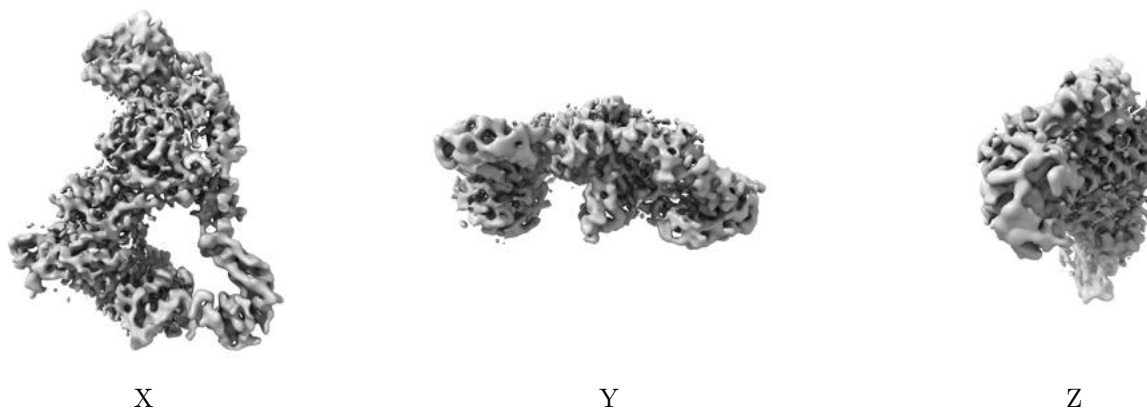


Z

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.

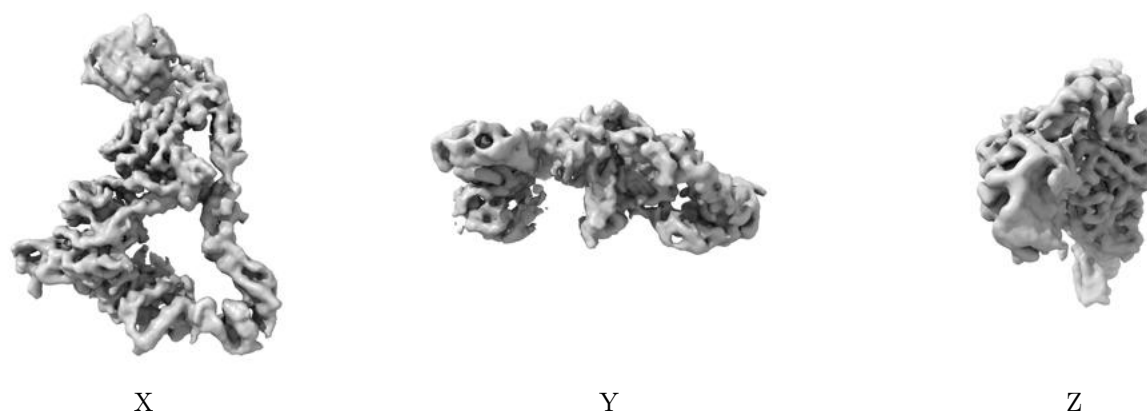
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.5. 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.

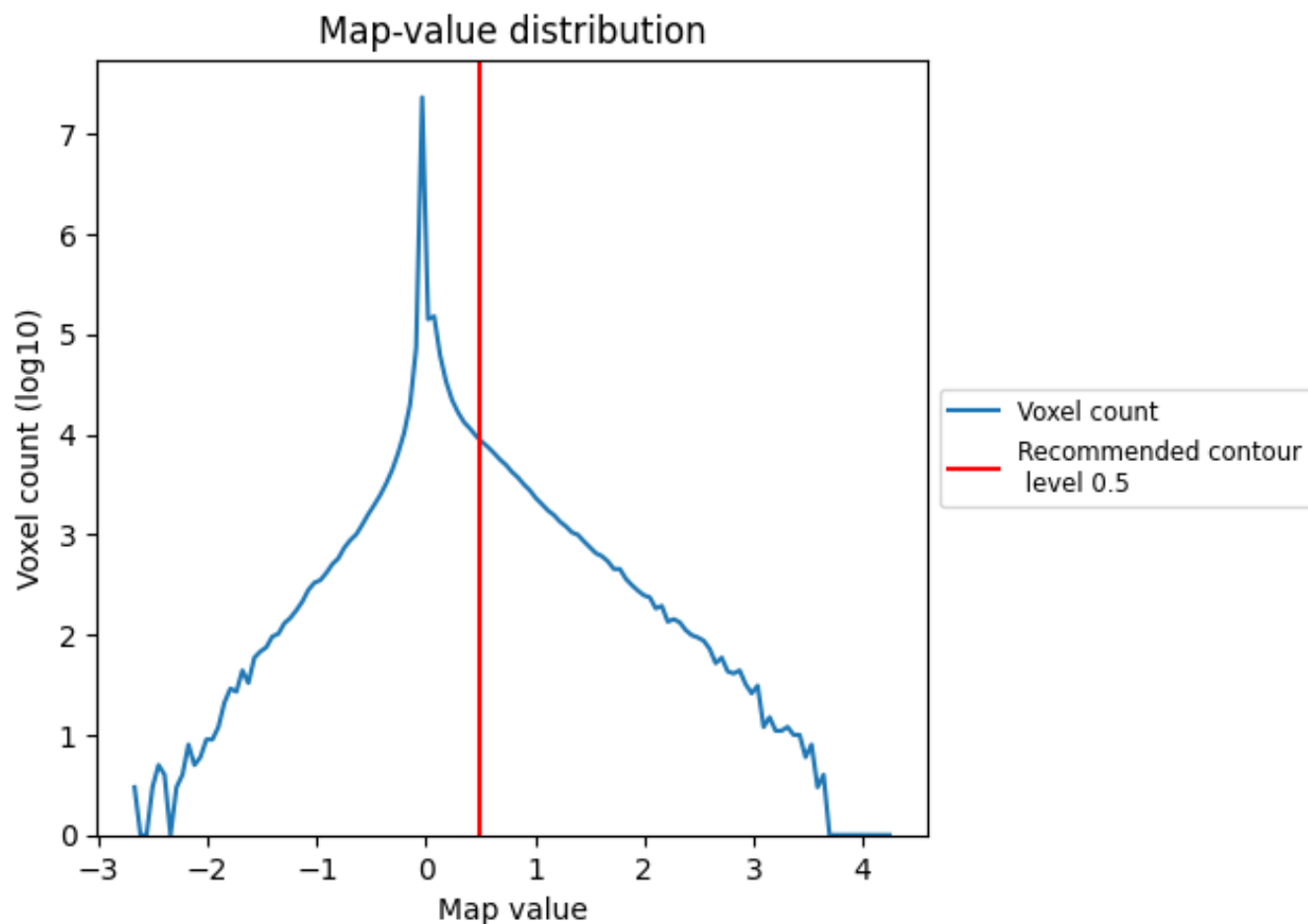
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

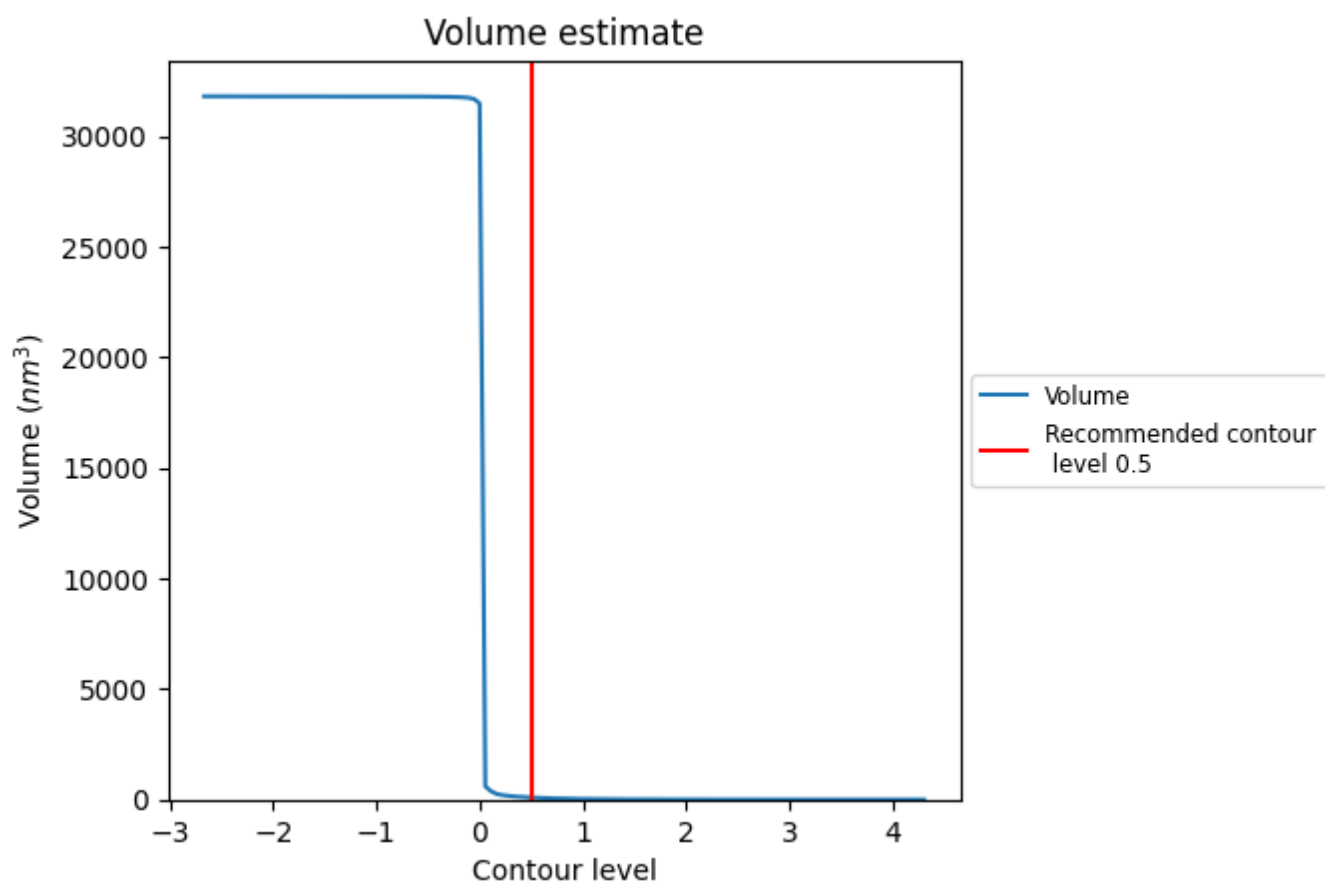
This section contains the results of statistical analysis of the map.

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.

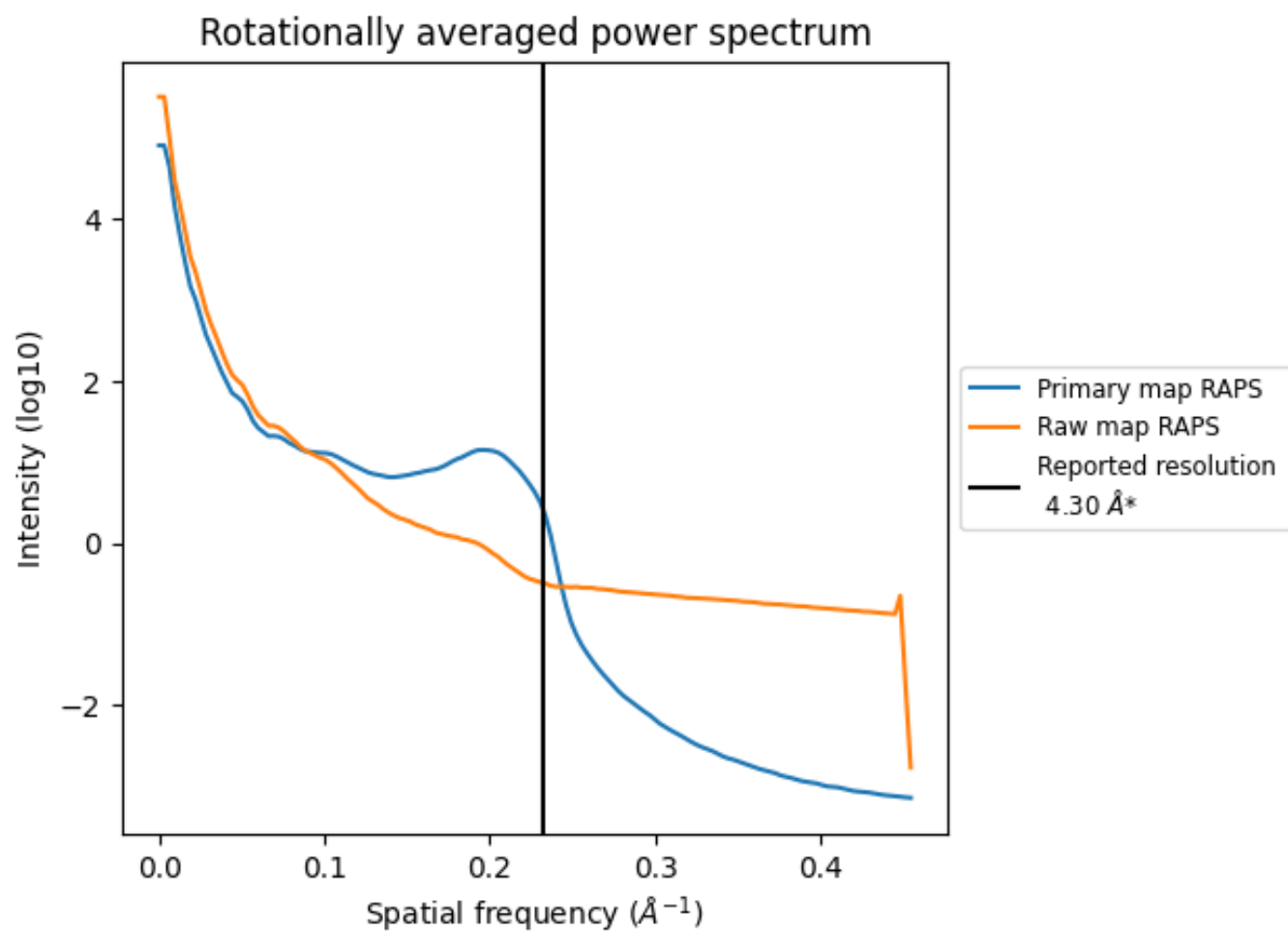
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 92 nm^3 ; this corresponds to an approximate mass of 83 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 ⓘ

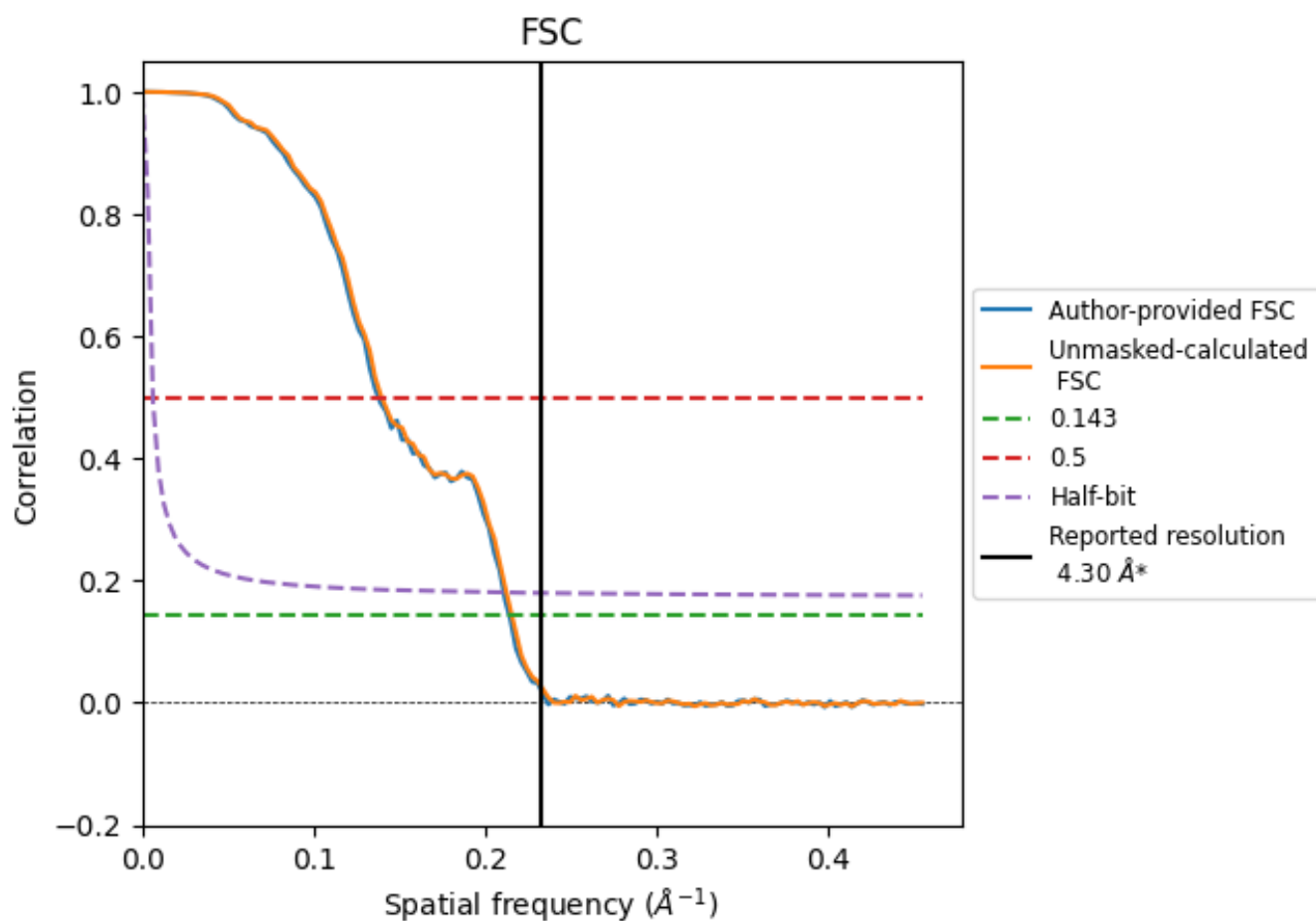


*Reported resolution corresponds to spatial frequency of 0.233 \AA^{-1}

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 0.233 Å⁻¹

8.2 Resolution estimates [i](#)

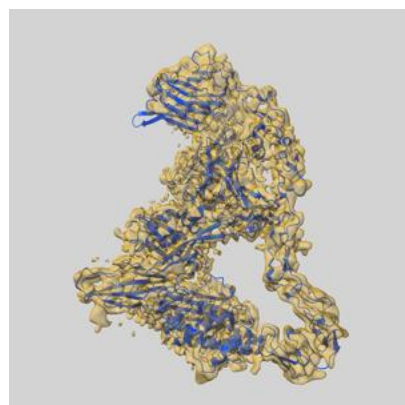
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.30	-	-
Author-provided FSC curve	4.68	7.27	4.75
Unmasked-calculated*	4.64	7.17	4.71

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

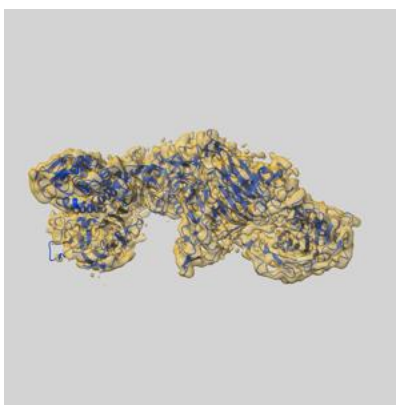
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-43644 and PDB model 8VY2. Per-residue inclusion information can be found in section [3](#) on page [5](#).

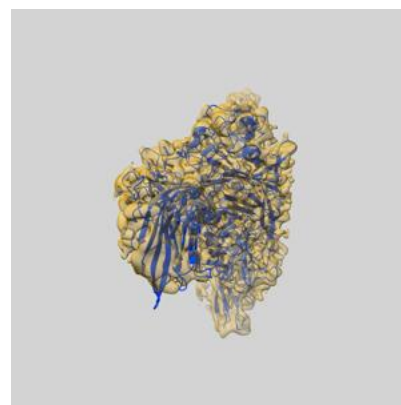
9.1 Map-model overlay [i](#)



X



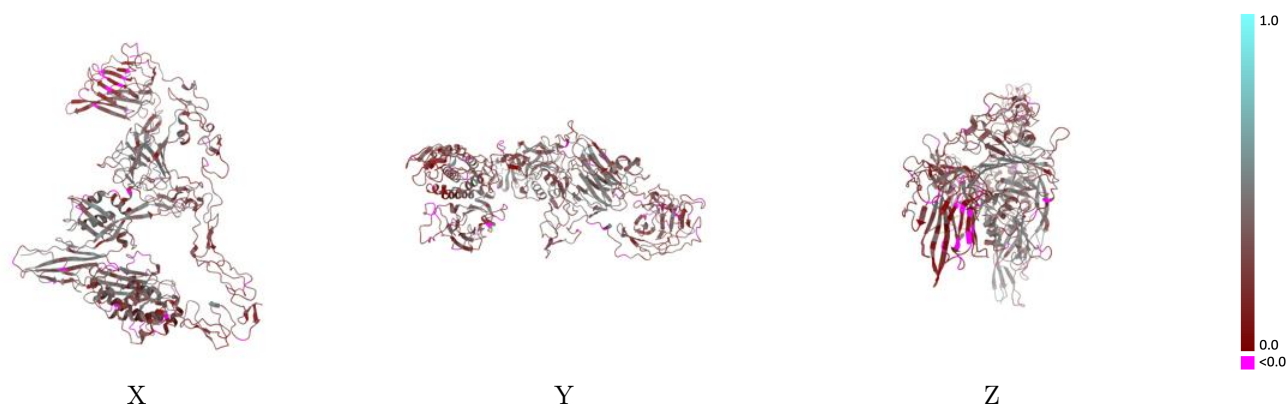
Y



Z

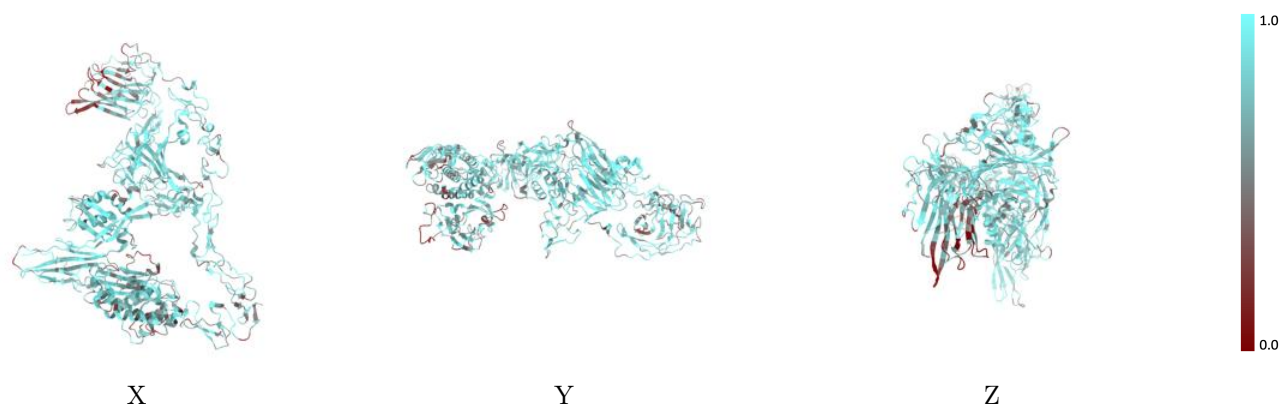
The images above show the 3D surface view of the map at the recommended contour level 0.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



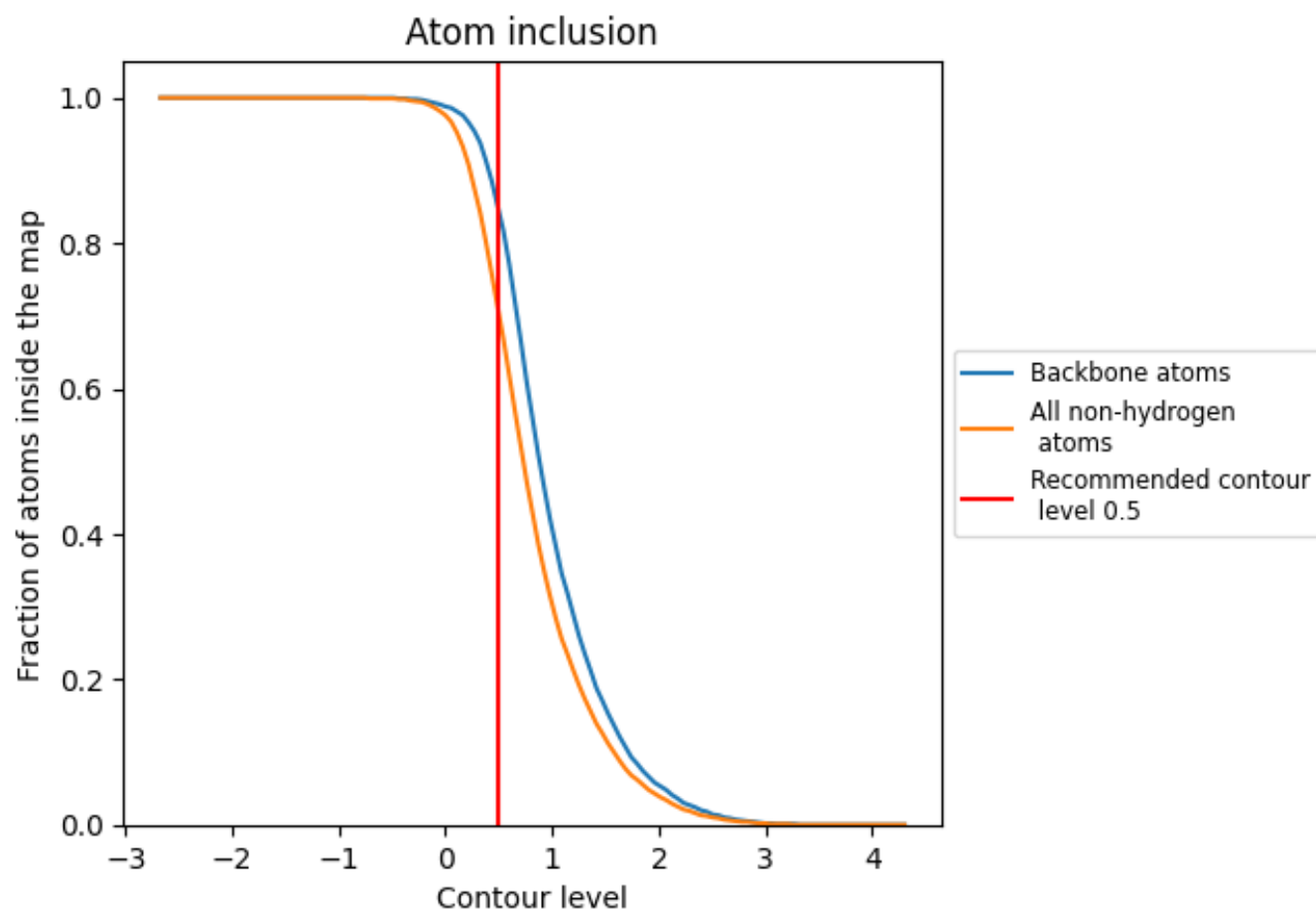
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.5).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 70% 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 (0.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7050	<div></div> 0.2960
A	<div></div> 0.7070	<div></div> 0.2940
B	<div></div> 0.6430	<div></div> 0.3790
C	<div></div> 0.5900	<div></div> 0.4180
D	<div></div> 0.4290	<div></div> 0.4860
E	<div></div> 0.6070	<div></div> 0.3570

