



Full wwPDB EM Validation Report ⓘ

Dec 12, 2022 – 03:29 PM EST

PDB ID : 8EDW
EMDB ID : EMD-28041
Title : Cryo-EM Structure of human ABCA7 in BPL/Ch Nanodiscs
Authors : Alam, A.; Le, L.T.M.; Thompson, J.R.
Deposited on : 2022-09-06
Resolution : 3.60 Å(reported)
Based on initial model : 6JBJ

This is a Full wwPDB EM Validation 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.dev43
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 : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

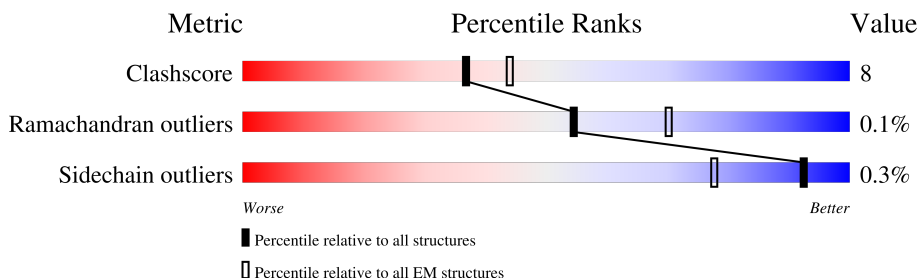
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.60 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	A	2146	<div> <div>16%</div> <div>68%</div> <div>16%</div> <div>16%</div> </div>
2	B	2	<div>100%</div>
2	D	2	<div>100%</div>

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 14321 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 Phospholipid-transporting ATPase ABCA7.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1804	Total	C	N	O	S	0	0
			13931	8963	2452	2453	63		

- 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	D	2	Total	C	N	O	0	0
			28	16	2	10		
2	B	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C₈H₁₅NO₆).

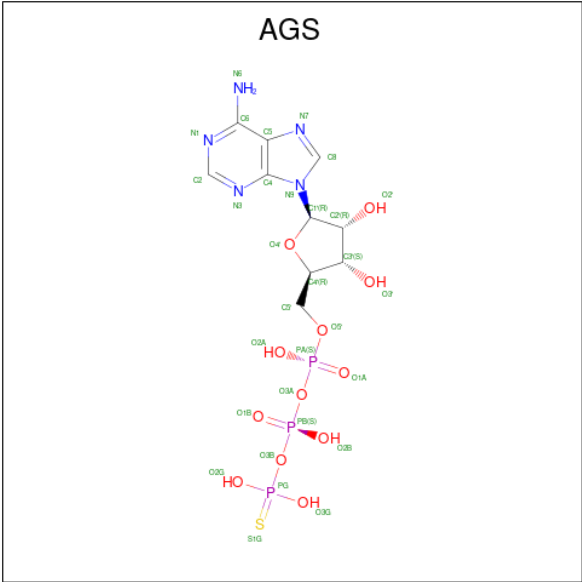


Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	
3	A	1	Total	C	N	O	0
			56	32	4	20	

- Molecule 4 is UNKNOWN LIGAND (three-letter code: UNL) (formula:) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
4	A	18	Total	C	0
			216	216	

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (three-letter code: AGS) (formula: $C_{10}H_{16}N_5O_{12}P_3S$).

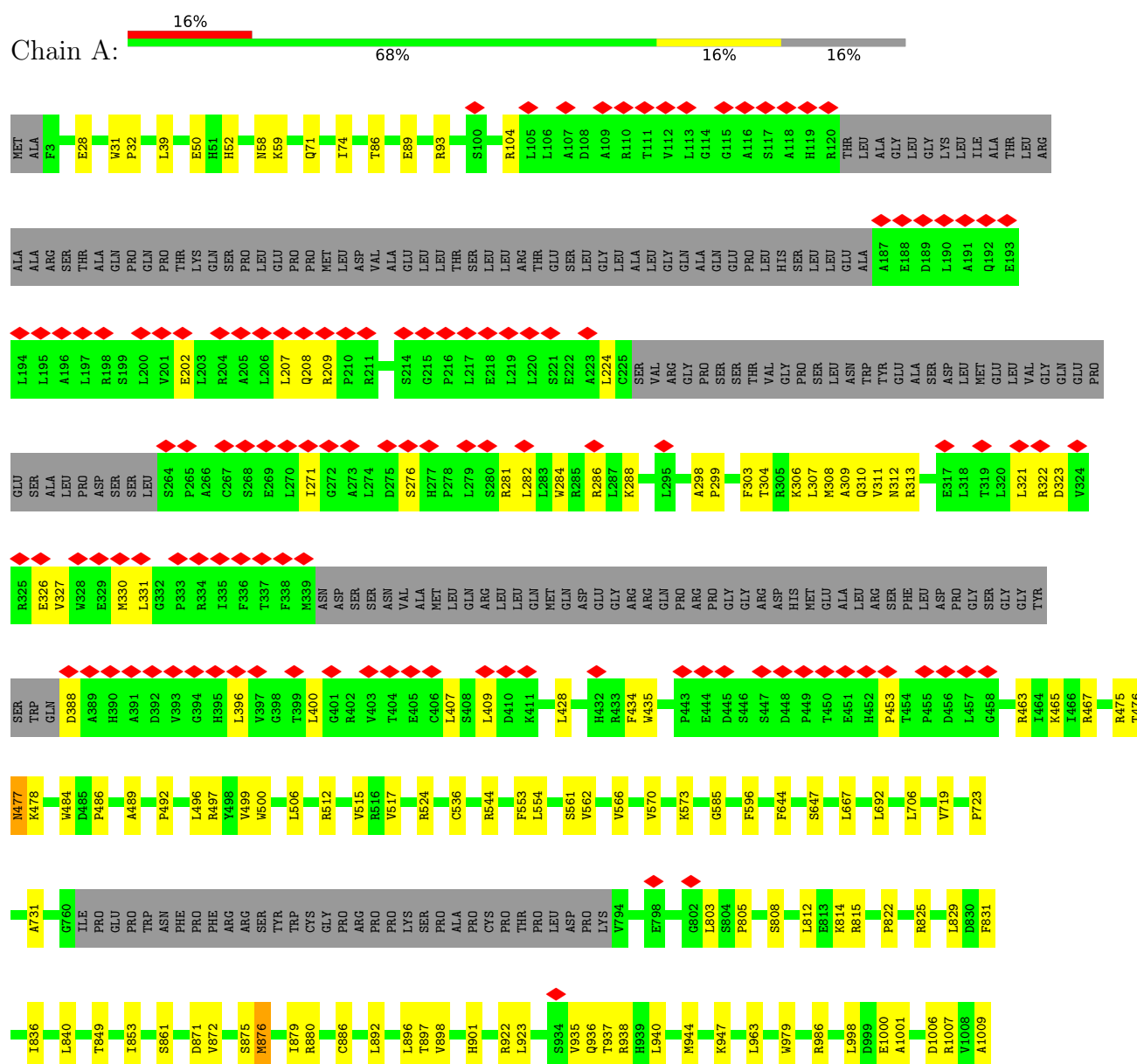


Mol	Chain	Residues	Atoms						AltConf
5	A	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	
5	A	1	Total	C	N	O	P	S	0
			62	20	10	24	6	2	

3 Residue-property plots [i](#)

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: Phospholipid-transporting ATPase ABCA7



GLU	S2031	S1908	M1907	V1729	L1651	A1545	L1443	K1329	I1243	LEU	R1090	R1015
ALA	Q2032	G1909	P1808	V1730	H1855	M1546	S1444	G1334	V1244	ASP	L1091	L1016
GLY	P2033	L1910	D1811	K1732	S1547	S1548	P1445	G1335	L1245	VAL	V1092	
VAL	A2034	A1911	H1812	N1733	F1549	V1549	L1446	W1336	P1246	LEU	E1093	C1019
ASP	A2035	A1919	H1813	L1734	F1553		P1447	E1339	F1249	LEU	E1094	L1023
PRO	A2036	D1920	L1814	L1735	R1561		G1448	G1342	V1250	LYS	P1096	R1027
ALA	P2037	P1921	C1815	L1736	V1562		G1449	S1343	G1251	PRO	H1087	L1028
PRO	A2038	A1922	L1815	A1736	R1562		L1450	P1345	L1252	GLN	E1098	L1029
GLY	A2039	L1923	P1818	A1737	H1567		L1451	Q1346	A1253	GLN	L1099	G1030
LEU	A2040	G1924	E1821	Q1740	K1566		L1452	C1347	L1254	THR	V1100	Y1034
GLN	G2044	Y1925	G1830	L1743	H1567		R1453	S1348		ALA	L1101	
HIS	A2045	Y1926	F1744	L1745	L1570		V1454	R1349	S1257	LEU	V1102	A1040
PRO	E2046	N1930	L1746	M1571	M1571		L1455	P1350	L1258	GLU	L1103	ARG
LYS	L2047	K1933	L1747	L1574	L1574		K1456	G1351		ASN	P1104	LEU
ARG	R2048	L1934	F1747	S1575	S1575		N1457	A1352	I1259	GLY	Y1105	PRO
VAL	E2049	V1941	L1748	L1576	L1576		L1458	R1353	V1260	GLU	F1113	LEU
GLN	G2052	G1942	L1749	F1672	F1672		T1459	L1356	P1261	PRO	F1117	THR
LEU	Q2058	A1945	Q1756	S1673	S1673		A1460	P1357		ALA		THR
ASP	L2059	V1946	L1756	D1674	D1674		A1462	P1357	G1264	GLY		ASN
PRO	P2060	F1947	L1757	K1676	K1676		H1462	D1358	H1265	GLU	D1121	GLU
THR	P2061	F1948	L1758	L1677	L1677		H1463	C1359	Y1266	LYS		LYS
ALA	G2062	L1949	L1759	E1678	E1678		S1464	P1360	P1267	ALA		ALA
THR	G2063	P1952	L1760	L1681	L1681		L1465	P1366	S1272	GLU	R1128	ASP
VAL	R2064	G1955	L1761	L1682	L1682		Q1468	P1367	M1275	THR	L1129	THR
LEU	C2065	M1956	L1762	L1683	L1683		D1469	P1369	A1287	GLY	T1130	ASP
GLY	A2066	L1957	L1763	L1684	L1684		S1470	Q1370		GLY	T1134	GLU
A2068	R2069	P1958	L1764	L1685	L1685		L1471	N1386	G1292	GLY	S1135	SER
V2070	G2071	H1959	L1765	Q1686	Q1686		M1477	L1387	R1293	PRO	D1136	VAL
L2074	H2077	R1961	L1766	L1687	L1687		L1478	K1403	A1294	ALA	T1137	ASP
		Y1965	L1767	L1688	L1688		P1500	K1404	R1295	VAL	S1138	THR
		L1968	L1768	L1689	L1689		P1503	L1405	A1299	GLY	L1139	ARG
		L1969	L1769	L1690	L1690		A1504	K1406		ARG	E1141	GLN
		A1970	L1770	L1691	L1691		R1505		A1299	VAL	F1142	GLU
		L1971	L1771	L1692	L1692		L1513		Q1302	GLN	F1143	LYS
		V1972	L1772	L1693	L1693		L1517			GLY	V1147	ASN
		V1973	L1773	L1694	L1694		T1520		Q1220	GLY		SER
		E1974	L1774	L1695	L1695		K1521		L1224	GLN	A1152	GLN
		C1987	L1775	L1696	L1696		E1522		K1227	SER	D1153	GLY
		E1988	L1776	L1697	L1697		Q1523		L1230	ARG	T1154	SER
		E1989	L1777	L1698	L1698		L1524			MET	D1155	ARG
		L1990	L1778	L1699	L1699		S1525		R1233	GLU	V1073	V1073
		L2006	L1779	L1700	L1700		E1526		R1234	ASP	G1074	G1074
		H2020	L1780	L1701	L1701		G1527		R1236	GLY	T1075	T1075
		A2029	L1781	L1702	L1702		A1528		R1237	SER	P1076	P1076
		R2030	L1782	L1703	L1703		M1530		R1238	CYS	Q1077	Q1077
			L1783	L1704	L1704		A1531		G1238	GLY	L1078	L1078
			L1784	L1705	L1705		S1532		H1084	HIS		
			L1785	L1706	L1706		V1533			LEU	P1087	P1087
			L1786	L1707	L1707		D1534			CYS	G1088	G1088
			L1787	L1708	L1708					THR	Y1089	Y1089
			L1788	L1709	L1709					GLY		
			L1789	L1710	L1710					ALA		
			L1790	L1711	L1711					GLY		
			L1791	L1712	L1712							
			L1792	L1713	L1713							
			L1793	L1714	L1714							
			L1794	L1715	L1715							
			L1795	L1716	L1716							
			L1796	L1717	L1717							
			L1797	L1718	L1718							
			L1798	L1719	L1719							
			L1799	L1720	L1720							
			L1800	L1721	L1721							
			L1801	L1722	L1722							
			L1802	L1723	L1723							
			L1803	L1724	L1724							
			L1804	L1725	L1725							
			L1805	L1726	L1726							
			L1806	L1727	L1727							
			L1807	L1728	L1728							

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

Chain D:  100%

MAG1
MAG2

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

Chain B:  100%

MAG1
MAG2

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	91381	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 ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2400	Depositor
Magnification	Not provided	
Image detector	FEI FALCON III (4k x 4k)	Depositor
Maximum map value	0.188	Depositor
Minimum map value	-0.143	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.018	Depositor
Map size (Å)	343.68, 343.68, 343.68	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.895, 0.895, 0.895	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: AGS, UNL, 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	0.25	0/14270	0.51	0/19416

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [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	A	13931	0	14109	238	0
2	B	28	0	25	0	0
2	D	28	0	25	0	0
3	A	56	0	52	1	0
4	A	216	0	0	0	0
5	A	62	0	24	3	0
All	All	14321	0	14235	238	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 8.

All (238) 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:897:THR:HG22	1:A:898:VAL:H	1.22	1.03
1:A:310:GLN:HA	1:A:313:ARG:HE	1.40	0.86
1:A:897:THR:HG22	1:A:898:VAL:N	1.87	0.86
1:A:897:THR:HG21	1:A:936:GLN:HA	1.60	0.84
1:A:897:THR:CG2	1:A:898:VAL:H	1.94	0.79
1:A:1499:LEU:HD12	1:A:1500:PRO:HD2	1.68	0.74
1:A:892:LEU:HD23	1:A:938:ARG:HD2	1.69	0.74
1:A:1499:LEU:HD23	1:A:1505:ARG:HD3	1.69	0.72
1:A:1343:PRO:HG3	1:A:1366:PRO:HD3	1.69	0.72
1:A:1090:ARG:HB3	1:A:1102:VAL:HB	1.71	0.72
1:A:1802:TYR:HE2	5:A:2224:AGS:H1'	1.56	0.68
1:A:1346:GLN:NE2	1:A:1359:CYS:O	2.27	0.67
1:A:897:THR:HG21	1:A:936:GLN:CA	2.24	0.67
1:A:897:THR:CG2	1:A:936:GLN:HA	2.26	0.65
1:A:897:THR:CG2	1:A:898:VAL:N	2.57	0.65
1:A:2046:GLU:HB2	1:A:2058:GLN:HB3	1.79	0.65
1:A:1830:GLY:HA2	5:A:2224:AGS:H5'1	1.78	0.64
1:A:1034:TYR:HB2	1:A:1135:SER:HB3	1.81	0.63
1:A:1888:LEU:HD11	1:A:1909:GLY:HA3	1.79	0.63
1:A:986:ARG:NH2	1:A:1006:ASP:OD2	2.31	0.63
1:A:271:ILE:HG23	1:A:284:TRP:HH2	1.64	0.62
1:A:309:ALA:HA	1:A:312:ASN:OD1	1.99	0.62
1:A:1776:VAL:HA	1:A:2006:LEU:HD23	1.81	0.62
1:A:979:TRP:NE1	1:A:1000:GLU:OE2	2.33	0.62
1:A:901:HIS:HB2	1:A:938:ARG:NH2	2.14	0.62
1:A:1293:ARG:NH2	1:A:1468:GLN:O	2.32	0.62
1:A:1965:TRP:HZ2	1:A:1987:GLU:HG2	1.65	0.61
1:A:58:ASN:OD1	1:A:59:LYS:N	2.33	0.61
1:A:1779:GLU:HA	1:A:1782:ARG:HG2	1.82	0.61
1:A:1885:ARG:NH1	1:A:1919:ALA:O	2.35	0.60
1:A:492:PRO:HA	1:A:496:LEU:HB2	1.83	0.60
1:A:1702:ASP:HB3	1:A:1729:VAL:HG13	1.84	0.59
1:A:1591:TYR:CZ	1:A:1627:GLY:HA3	2.37	0.59
1:A:489:ALA:O	1:A:1477:ASN:ND2	2.36	0.59
1:A:104:ARG:NH2	1:A:202:GLU:OE1	2.35	0.59
1:A:840:LEU:HD21	1:A:1001:ALA:HB2	1.85	0.59
1:A:2090:GLN:H	1:A:2092:MET:HE2	1.67	0.58
1:A:544:ARG:HD3	1:A:1406:LYS:HD2	1.84	0.58
1:A:321:LEU:HD13	1:A:400:LEU:HD11	1.84	0.58
1:A:570:VAL:HG13	1:A:573:LYS:HZ1	1.69	0.58
1:A:28:GLU:OE2	1:A:561:SER:OG	2.21	0.58
1:A:1798:LEU:HB3	1:A:1813:LEU:HB3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1224:LEU:O	1:A:1227:LYS:HG3	2.04	0.57
1:A:1307:GLU:HG3	1:A:1309:PRO:HD2	1.87	0.57
1:A:871:ASP:OD1	1:A:872:VAL:N	2.38	0.57
1:A:1682:ARG:NH1	1:A:1686:GLN:OE1	2.35	0.57
1:A:1134:ILE:HG22	1:A:2090:GLN:HB3	1.87	0.56
1:A:1137:THR:OG1	1:A:1141:GLU:OE2	2.22	0.56
1:A:1632:PRO:HB2	1:A:1744:PHE:HB2	1.86	0.56
1:A:1636:PRO:HG3	1:A:1748:THR:HB	1.86	0.56
1:A:1356:LEU:HB3	1:A:1357:PRO:HD3	1.87	0.56
1:A:937:THR:HG21	1:A:940:LEU:HD22	1.87	0.56
1:A:1243:ILE:HG23	1:A:1594:PRO:HG3	1.88	0.56
1:A:2044:GLY:HA3	1:A:2060:PRO:HD3	1.88	0.56
1:A:435:TRP:CH2	1:A:506:LEU:HD11	2.42	0.55
1:A:477:ASN:C	1:A:477:ASN:HD22	2.08	0.55
1:A:1009:ALA:HB1	1:A:1016:LEU:HD11	1.89	0.55
1:A:1561:ARG:HG3	1:A:1566:LYS:HE2	1.89	0.55
1:A:1609:ALA:O	1:A:1707:GLN:NE2	2.40	0.54
1:A:1561:ARG:HA	1:A:1566:LYS:HD3	1.87	0.54
1:A:1117:PHE:HB2	1:A:2068:ALA:HB2	1.88	0.54
1:A:876:MET:O	1:A:880:ARG:NH1	2.40	0.54
1:A:1088:GLY:HA3	1:A:1104:PRO:HG3	1.89	0.54
1:A:1921:ARG:NH1	1:A:1925:THR:OG1	2.41	0.54
1:A:310:GLN:HA	1:A:313:ARG:NE	2.16	0.53
1:A:1220:GLN:NE2	1:A:1574:LEU:HA	2.22	0.53
1:A:897:THR:HG21	1:A:936:GLN:HG2	1.91	0.53
1:A:1868:SER:HB2	1:A:1945:ALA:H	1.74	0.52
1:A:570:VAL:HA	1:A:573:LYS:HG2	1.91	0.52
1:A:812:LEU:HD21	1:A:853:ILE:HG21	1.92	0.52
1:A:814:LYS:HA	1:A:861:SER:HB2	1.91	0.52
1:A:1883:THR:HA	1:A:1923:ALA:H	1.73	0.52
1:A:284:TRP:CE2	1:A:288:LYS:HE3	2.44	0.52
1:A:1970:ALA:O	1:A:1974:GLU:HG2	2.10	0.52
1:A:407:LEU:HG	1:A:409:LEU:H	1.74	0.52
1:A:475:ARG:HH21	1:A:478:LYS:HG2	1.76	0.51
1:A:825:ARG:HH11	1:A:1015:ARG:HH21	1.57	0.51
1:A:849:THR:O	1:A:853:ILE:HG12	2.09	0.51
1:A:39:LEU:HD13	1:A:553:PHE:HE2	1.73	0.51
1:A:330:MET:SD	1:A:331:LEU:HD12	2.51	0.51
1:A:1591:TYR:CE2	1:A:1627:GLY:HA3	2.46	0.51
1:A:1968:LEU:HA	1:A:1971:VAL:HG12	1.92	0.51
1:A:327:VAL:HA	1:A:330:MET:HG3	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:SER:HB2	1:A:879:ILE:HB	1.92	0.51
1:A:815:ARG:HG2	1:A:822:PRO:HB3	1.92	0.51
1:A:1272:SER:O	1:A:1275:MET:HG2	2.10	0.51
1:A:1969:LEU:HA	1:A:1972:VAL:HG12	1.93	0.51
1:A:428:LEU:HB2	1:A:434:PHE:HB2	1.92	0.50
1:A:1302:GLN:NE2	1:A:1307:GLU:O	2.24	0.50
1:A:304:THR:O	1:A:308:MET:HE2	2.11	0.50
1:A:477:ASN:C	1:A:477:ASN:ND2	2.64	0.50
1:A:497:ARG:HA	1:A:500:TRP:NE1	2.26	0.50
1:A:467:ARG:HB3	1:A:1517:LEU:HG	1.92	0.50
1:A:1690:ILE:O	1:A:1740:GLN:NE2	2.38	0.50
1:A:284:TRP:CD1	1:A:288:LYS:HG3	2.47	0.50
1:A:86:THR:OG1	1:A:89:GLU:OE1	2.29	0.50
1:A:1833:LYS:NZ	5:A:2224:AGS:O2B	2.35	0.50
1:A:585:GLY:HA2	1:A:880:ARG:HH21	1.76	0.50
1:A:282:LEU:O	1:A:286:ARG:HG2	2.12	0.49
1:A:803:LEU:HD23	1:A:805:PRO:HD3	1.93	0.49
1:A:1883:THR:HG22	1:A:1922:PRO:HA	1.93	0.49
1:A:1872:CYS:HB3	1:A:1949:LEU:HG	1.94	0.49
1:A:1529:LEU:HD11	1:A:1670:GLU:HG2	1.93	0.49
1:A:1591:TYR:O	1:A:1594:PRO:HD2	2.12	0.48
1:A:1729:VAL:HG12	1:A:1730:VAL:HG13	1.94	0.48
1:A:307:LEU:HD12	1:A:517:VAL:HG21	1.95	0.48
1:A:2074:LEU:HA	1:A:2077:HIS:HB2	1.95	0.48
1:A:1795:LEU:HD13	1:A:1815:LEU:HB3	1.96	0.48
1:A:998:LEU:HD21	1:A:1143:PHE:CE2	2.49	0.48
1:A:307:LEU:O	1:A:311:VAL:HG23	2.14	0.48
1:A:1792:VAL:HG12	1:A:1793:LEU:HD12	1.96	0.48
1:A:1727:TRP:HA	1:A:1731:GLY:HA3	1.95	0.48
1:A:1853:LEU:HD11	1:A:1946:VAL:HG11	1.95	0.48
1:A:1312:GLN:O	1:A:1316:HIS:ND1	2.47	0.47
1:A:1861:GLU:OE2	1:A:1864:ALA:HB3	2.14	0.47
1:A:1921:ARG:HB2	1:A:1926:TYR:HE1	1.78	0.47
1:A:1802:TYR:HH	1:A:1835:SER:HG	1.63	0.47
1:A:1883:THR:O	1:A:1887:HIS:ND1	2.47	0.47
1:A:207:LEU:HD21	1:A:396:LEU:HD22	1.95	0.47
1:A:59:LYS:HE3	1:A:499:VAL:HG11	1.97	0.47
1:A:512:ARG:HA	1:A:515:VAL:HG12	1.97	0.47
1:A:1553:PHE:CD2	1:A:1587:ASP:HB2	2.50	0.47
1:A:1808:PRO:HB2	1:A:1811:ASP:HB2	1.96	0.47
1:A:1888:LEU:HD22	1:A:1906:ALA:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1682:ARG:HA	1:A:1685:LYS:HE2	1.96	0.47
1:A:323:ASP:O	1:A:326:GLU:HG3	2.14	0.46
1:A:922:ARG:HE	1:A:923:LEU:HD12	1.80	0.46
1:A:1349:ARG:HG2	1:A:1351:GLY:H	1.80	0.46
1:A:596:PHE:HD1	1:A:644:PHE:HE2	1.63	0.46
1:A:1403:LEU:HD22	1:A:1406:LYS:HZ3	1.81	0.46
1:A:465:LYS:HE2	1:A:1513:LEU:HD22	1.98	0.46
1:A:1347:CYS:SG	1:A:1359:CYS:N	2.85	0.46
1:A:836:ILE:HD11	1:A:986:ARG:HB2	1.97	0.46
1:A:1865:ALA:O	1:A:1869:MET:HG3	2.15	0.46
1:A:1683:ILE:HG13	1:A:1686:GLN:NE2	2.31	0.46
1:A:1882:LEU:HD23	1:A:1886:GLU:HG3	1.98	0.46
1:A:822:PRO:HG2	1:A:825:ARG:HG2	1.98	0.46
1:A:1321:PRO:HD2	1:A:1368:PRO:HB2	1.98	0.46
1:A:1740:GLN:O	1:A:1743:LEU:HG	2.16	0.46
1:A:1588:MET:HE3	1:A:1628:TRP:CD1	2.51	0.46
1:A:1709:MET:O	1:A:1713:PHE:HB2	2.16	0.46
1:A:944:MET:O	1:A:947:LYS:HB3	2.16	0.45
1:A:1520:THR:O	1:A:1524:LEU:N	2.39	0.45
1:A:1588:MET:O	1:A:1592:LEU:HG	2.17	0.45
1:A:1958:PRO:HA	1:A:1961:ARG:HG2	1.99	0.45
1:A:562:VAL:O	1:A:566:VAL:HG12	2.16	0.45
1:A:1440:TRP:HB2	1:A:1455:LEU:HD13	1.98	0.45
1:A:1930:ASN:HA	1:A:1933:LYS:HG2	1.99	0.45
1:A:1965:TRP:CZ2	1:A:1987:GLU:HG2	2.49	0.45
1:A:1103:LEU:HD23	1:A:1113:PHE:CE1	2.51	0.45
1:A:1907:GLY:O	1:A:1911:ALA:N	2.47	0.45
1:A:1320:ALA:HB2	1:A:1370:GLN:HG3	1.99	0.45
1:A:524:ARG:HH12	1:A:1464:SER:HB2	1.82	0.45
1:A:1553:PHE:HE1	1:A:1590:ASN:HD22	1.63	0.45
1:A:276:SER:O	1:A:281:ARG:NH2	2.36	0.45
1:A:897:THR:HG22	1:A:898:VAL:HG22	1.98	0.45
1:A:31:TRP:HB3	1:A:32:PRO:HD3	1.99	0.45
1:A:298:ALA:HB3	1:A:299:PRO:HD3	1.99	0.45
1:A:484:TRP:CZ3	1:A:486:PRO:HG3	2.53	0.44
1:A:1293:ARG:HE	1:A:1469:ASP:HB3	1.81	0.44
1:A:1949:LEU:HD23	1:A:1952:PRO:HB3	1.98	0.44
1:A:1698:ARG:NH2	1:A:1733:ASN:OD1	2.49	0.44
1:A:303:PHE:HA	1:A:306:LYS:HD3	1.99	0.44
1:A:814:LYS:HD2	1:A:853:ILE:HD11	2.00	0.44
1:A:1342:SER:HB2	1:A:1343:PRO:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1678:GLN:O	1:A:1681:SER:HB3	2.17	0.44
1:A:1027:ARG:HD3	1:A:1027:ARG:HA	1.76	0.44
1:A:1553:PHE:CE2	1:A:1587:ASP:HB2	2.53	0.44
1:A:1776:VAL:HG22	1:A:2006:LEU:HB3	2.00	0.44
1:A:1818:PRO:HG2	1:A:1821:GLU:HG2	1.99	0.44
1:A:1863:SER:O	1:A:1867:LEU:HG	2.18	0.44
1:A:286:ARG:HD2	1:A:500:TRP:HB2	2.00	0.44
1:A:50:GLU:HB2	1:A:1349:ARG:NH2	2.33	0.44
1:A:1135:SER:HA	1:A:2092:MET:SD	2.58	0.44
1:A:1566:LYS:O	1:A:1570:LEU:HD23	2.17	0.44
1:A:1597:ILE:O	1:A:1600:LEU:HG	2.18	0.44
1:A:322:ARG:HH22	1:A:407:LEU:HD23	1.83	0.43
1:A:1404:LYS:HE2	1:A:1404:LYS:HB3	1.90	0.43
1:A:896:LEU:O	1:A:938:ARG:NE	2.52	0.43
1:A:1317:ARG:HD2	1:A:1317:ARG:HA	1.86	0.43
1:A:2034:ALA:HA	1:A:2037:PHE:HE1	1.83	0.43
1:A:1965:TRP:CD1	1:A:1991:LEU:HD11	2.54	0.43
1:A:1220:GLN:HE22	1:A:1574:LEU:HA	1.84	0.43
1:A:271:ILE:HG12	1:A:284:TRP:CZ2	2.53	0.43
1:A:897:THR:HG21	1:A:936:GLN:CB	2.48	0.43
1:A:1135:SER:HA	1:A:2092:MET:HE1	2.00	0.43
1:A:1793:LEU:HD21	1:A:1948:PHE:HZ	1.84	0.43
1:A:1864:ALA:HA	1:A:1867:LEU:HD12	2.00	0.43
1:A:1007:ARG:NH2	1:A:1019:CYS:HB2	2.33	0.43
1:A:1350:PRO:HD2	1:A:1353:ARG:O	2.19	0.43
1:A:310:GLN:O	1:A:313:ARG:HG2	2.19	0.42
1:A:706:LEU:HD22	1:A:723:PRO:HB2	2.01	0.42
1:A:475:ARG:CZ	1:A:477:ASN:HB3	2.49	0.42
1:A:1903:ALA:O	1:A:1906:ALA:HB3	2.19	0.42
1:A:2067:LEU:O	1:A:2070:VAL:HG12	2.19	0.42
1:A:1265:HIS:O	1:A:1267:PRO:HD3	2.19	0.42
1:A:208:GLN:NE2	1:A:388:ASP:OD2	2.53	0.42
1:A:886:CYS:HB3	1:A:963:LEU:HD23	2.01	0.42
1:A:719:VAL:HG12	1:A:731:ALA:HB2	2.01	0.42
1:A:1898:PRO:O	1:A:1902:VAL:HG23	2.19	0.42
1:A:497:ARG:HA	1:A:500:TRP:HE1	1.85	0.42
1:A:1775:ASP:HA	1:A:1778:ARG:HG2	2.01	0.42
1:A:453:PRO:O	1:A:463:ARG:NH2	2.53	0.42
1:A:1023:LEU:O	1:A:1027:ARG:HG2	2.20	0.42
1:A:1366:PRO:HB2	1:A:1367:PRO:HD3	2.00	0.42
1:A:1793:LEU:HD21	1:A:1948:PHE:CZ	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1969:LEU:O	1:A:1973:ARG:HD3	2.20	0.42
1:A:1246:PRO:HB3	1:A:1545:ALA:HB1	2.02	0.42
1:A:554:LEU:HD12	1:A:554:LEU:HA	1.77	0.41
1:A:1143:PHE:O	1:A:1147:VAL:HG23	2.20	0.41
1:A:1324:PRO:HG2	1:A:1327:VAL:HB	2.02	0.41
1:A:1432:LEU:HD22	1:A:1462:ALA:HB2	2.01	0.41
1:A:1676:LYS:HA	1:A:1676:LYS:HD3	1.75	0.41
1:A:935:VAL:HG23	1:A:937:THR:HG23	2.00	0.41
1:A:1546:MET:O	1:A:1546:MET:HG3	2.20	0.41
1:A:805:PRO:HB2	1:A:808:SER:OG	2.19	0.41
1:A:1469:ASP:OD1	1:A:1469:ASP:N	2.52	0.41
1:A:1702:ASP:O	1:A:1705:ARG:HG3	2.20	0.41
1:A:1302:GLN:HG2	1:A:1308:GLU:HA	2.02	0.41
1:A:1587:ASP:OD1	1:A:1588:MET:N	2.53	0.41
1:A:1260:VAL:HA	1:A:1261:PRO:HD3	1.90	0.41
1:A:476:THR:HG22	1:A:476:THR:O	2.20	0.41
1:A:209:ARG:HD3	1:A:209:ARG:HA	1.86	0.41
1:A:667:LEU:HB3	1:A:692:LEU:HD23	2.01	0.41
1:A:1386:ASN:O	1:A:1387:LEU:HB2	2.20	0.41
1:A:1567:HIS:CE1	1:A:1571:MET:SD	3.14	0.41
1:A:74:ILE:HG21	1:A:224:LEU:HD13	2.03	0.41
1:A:1230:LEU:O	1:A:1234:ARG:HG2	2.20	0.41
1:A:1669:LEU:O	1:A:1673:SER:OG	2.20	0.41
1:A:566:VAL:HG23	1:A:647:SER:OG	2.21	0.40
1:A:1230:LEU:HD12	1:A:1234:ARG:HH12	1.86	0.40
1:A:93:ARG:HD3	3:A:2202:NAG:H81	2.04	0.40
1:A:1470:SER:OG	1:A:1471:LEU:N	2.53	0.40
1:A:52:HIS:HA	1:A:536:CYS:SG	2.61	0.40
1:A:71:GLN:HG3	1:A:224:LEU:HB3	2.02	0.40
1:A:829:LEU:HD23	1:A:831:PHE:HE1	1.85	0.40
1:A:840:LEU:HD21	1:A:1001:ALA:CB	2.51	0.40
1:A:1245:LEU:HD23	1:A:1245:LEU:HA	1.93	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	1786/2146 (83%)	1711 (96%)	74 (4%)	1 (0%)	51 83

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	876	MET

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	1479/1764 (84%)	1475 (100%)	4 (0%)	92 97

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	477	ASN
1	A	1227	LYS
1	A	1295	ARG
1	A	1973	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1220	GLN
1	A	1346	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 ⓘ

4 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	1,2	14,14,15	0.28	0	17,19,21	0.66	0
2	NAG	B	2	2	14,14,15	0.33	0	17,19,21	0.74	0
2	NAG	D	1	1,2	14,14,15	0.27	0	17,19,21	0.92	1 (5%)
2	NAG	D	2	2	14,14,15	0.34	0	17,19,21	0.73	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	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	D	2	2	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C1-O5-C5	2.83	116.03	112.19
2	D	2	NAG	C1-O5-C5	2.19	115.15	112.19

There are no chirality outliers.

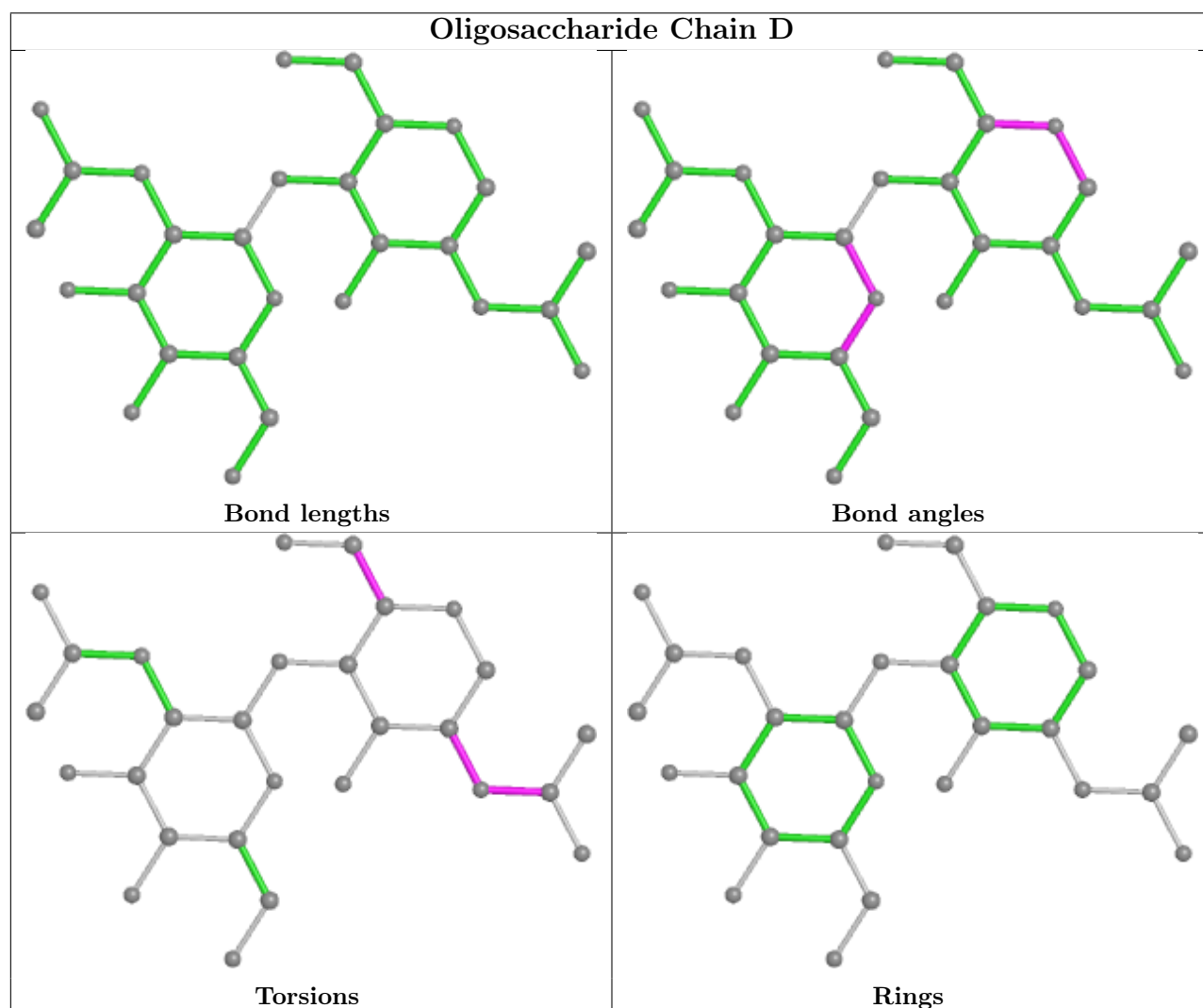
All (5) torsion outliers are listed below:

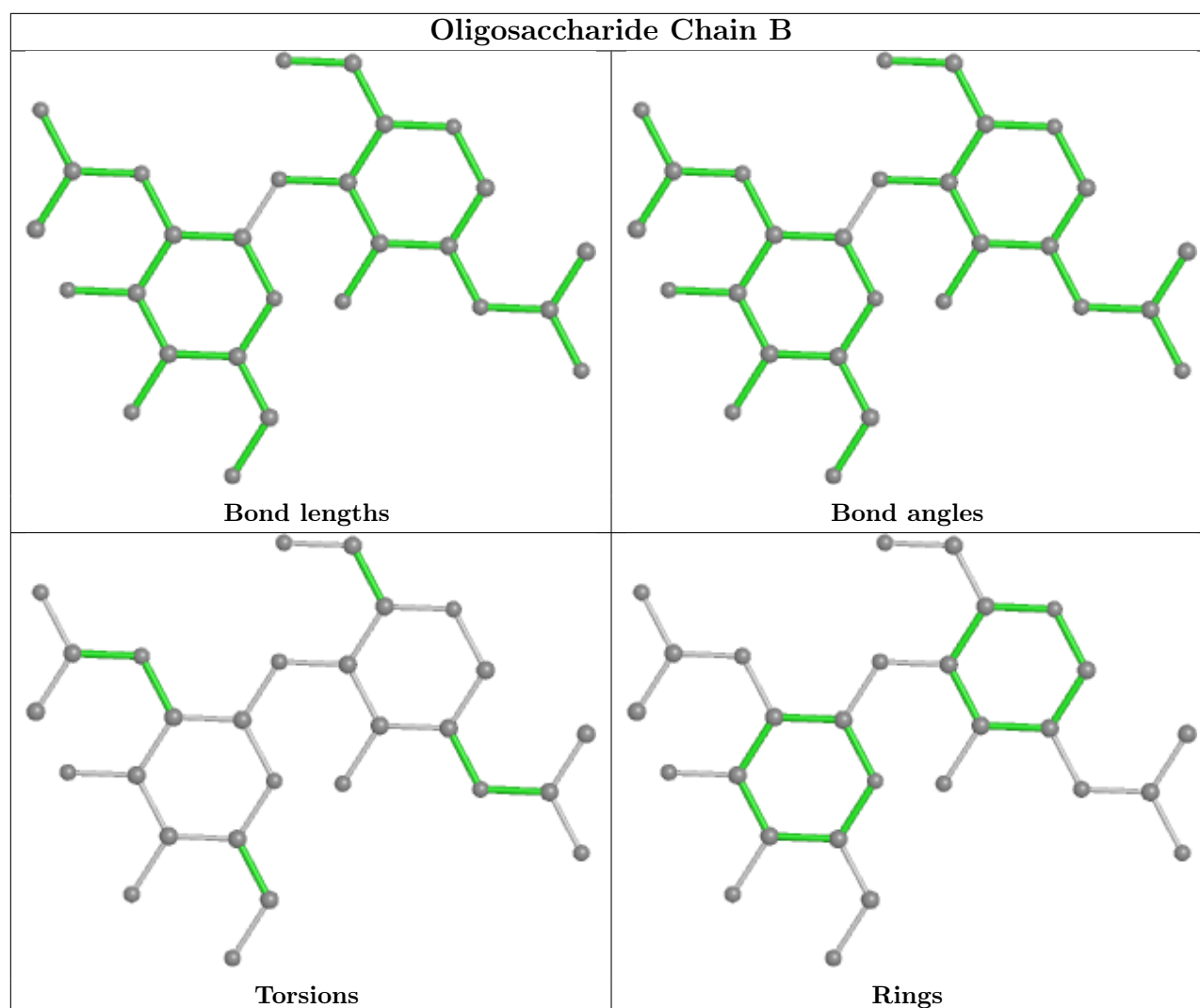
Mol	Chain	Res	Type	Atoms
2	D	1	NAG	C3-C2-N2-C7
2	D	1	NAG	C8-C7-N2-C2
2	D	1	NAG	O7-C7-N2-C2
2	D	1	NAG	C4-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

Of 24 ligands modelled in this entry, 18 are unknown - leaving 6 for Mogul analysis.

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	$\# Z > 2$
5	AGS	A	2224	-	26,33,33	0.82	1 (3%)	26,52,52	0.95	2 (7%)
3	NAG	A	2204	1	14,14,15	0.30	0	17,19,21	0.67	0
3	NAG	A	2203	1	14,14,15	0.35	0	17,19,21	1.40	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	A	2202	1	14,14,15	0.31	0	17,19,21	0.64	0
3	NAG	A	2201	1	14,14,15	0.29	0	17,19,21	0.61	0
5	AGS	A	2223	-	26,33,33	0.82	1 (3%)	26,52,52	0.91	2 (7%)

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
5	AGS	A	2224	-	-	3/17/38/38	0/3/3/3
3	NAG	A	2204	1	-	3/6/23/26	0/1/1/1
3	NAG	A	2203	1	-	4/6/23/26	0/1/1/1
3	NAG	A	2202	1	-	2/6/23/26	0/1/1/1
3	NAG	A	2201	1	-	1/6/23/26	0/1/1/1
5	AGS	A	2223	-	-	3/17/38/38	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2224	AGS	PG-S1G	2.14	1.95	1.90
5	A	2223	AGS	PG-S1G	2.12	1.95	1.90

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2203	NAG	C1-O5-C5	-4.54	106.04	112.19
3	A	2203	NAG	O5-C5-C6	2.86	111.69	107.20
5	A	2224	AGS	O4'-C1'-C2'	-2.38	103.44	106.93
5	A	2224	AGS	C5-C6-N6	2.25	123.78	120.35
5	A	2223	AGS	O4'-C1'-C2'	-2.25	103.64	106.93
5	A	2223	AGS	C5-C6-N6	2.24	123.76	120.35

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2223	AGS	C5'-O5'-PA-O1A
5	A	2223	AGS	C4'-C5'-O5'-PA
5	A	2224	AGS	C4'-C5'-O5'-PA

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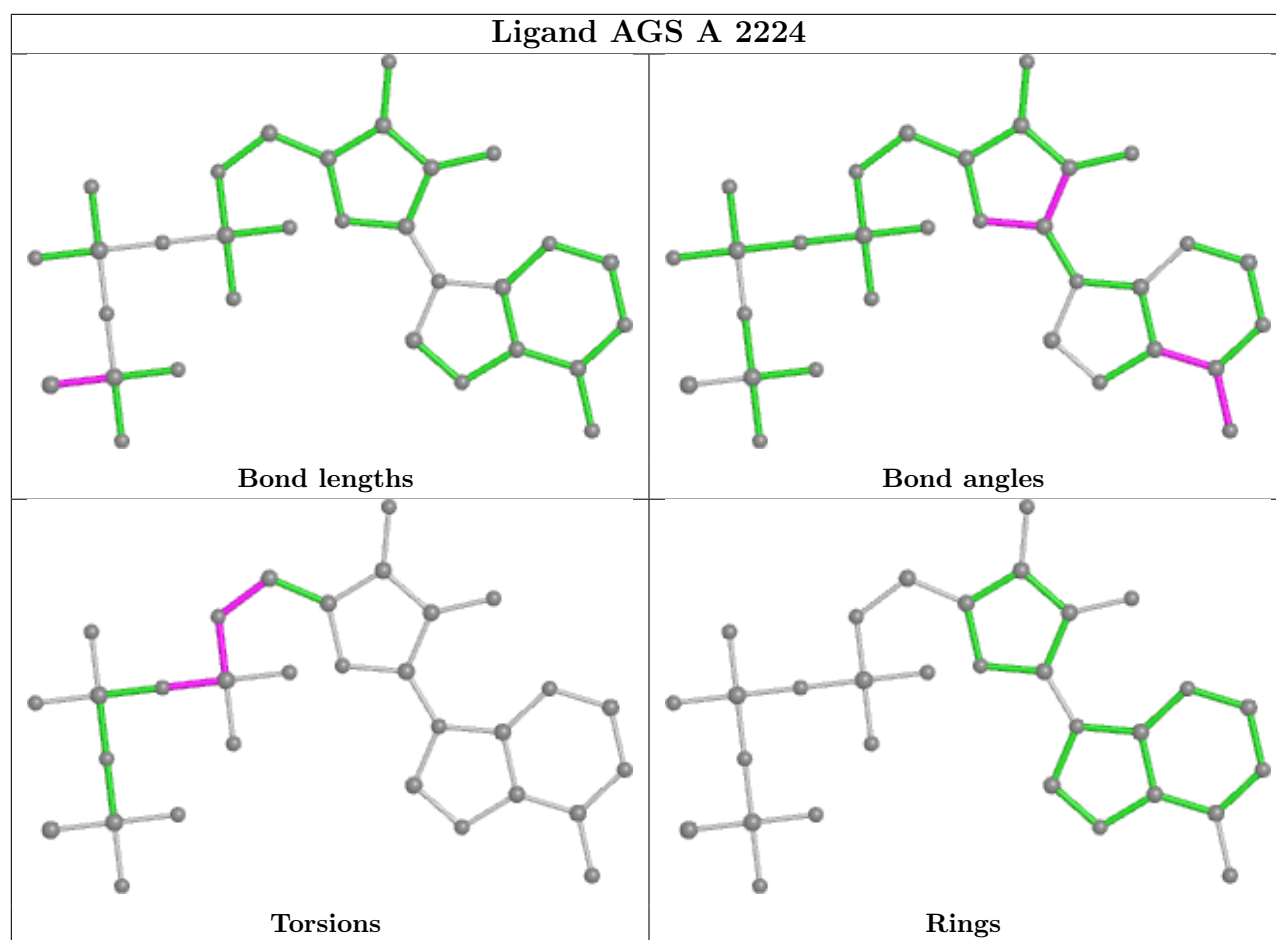
Mol	Chain	Res	Type	Atoms
3	A	2203	NAG	C8-C7-N2-C2
3	A	2203	NAG	O7-C7-N2-C2
3	A	2203	NAG	C4-C5-C6-O6
3	A	2202	NAG	C8-C7-N2-C2
3	A	2201	NAG	O5-C5-C6-O6
3	A	2204	NAG	O5-C5-C6-O6
3	A	2203	NAG	O5-C5-C6-O6
3	A	2202	NAG	O7-C7-N2-C2
5	A	2224	AGS	PB-O3A-PA-O5'
3	A	2204	NAG	C8-C7-N2-C2
3	A	2204	NAG	O7-C7-N2-C2
5	A	2223	AGS	C5'-O5'-PA-O3A
5	A	2224	AGS	C5'-O5'-PA-O3A

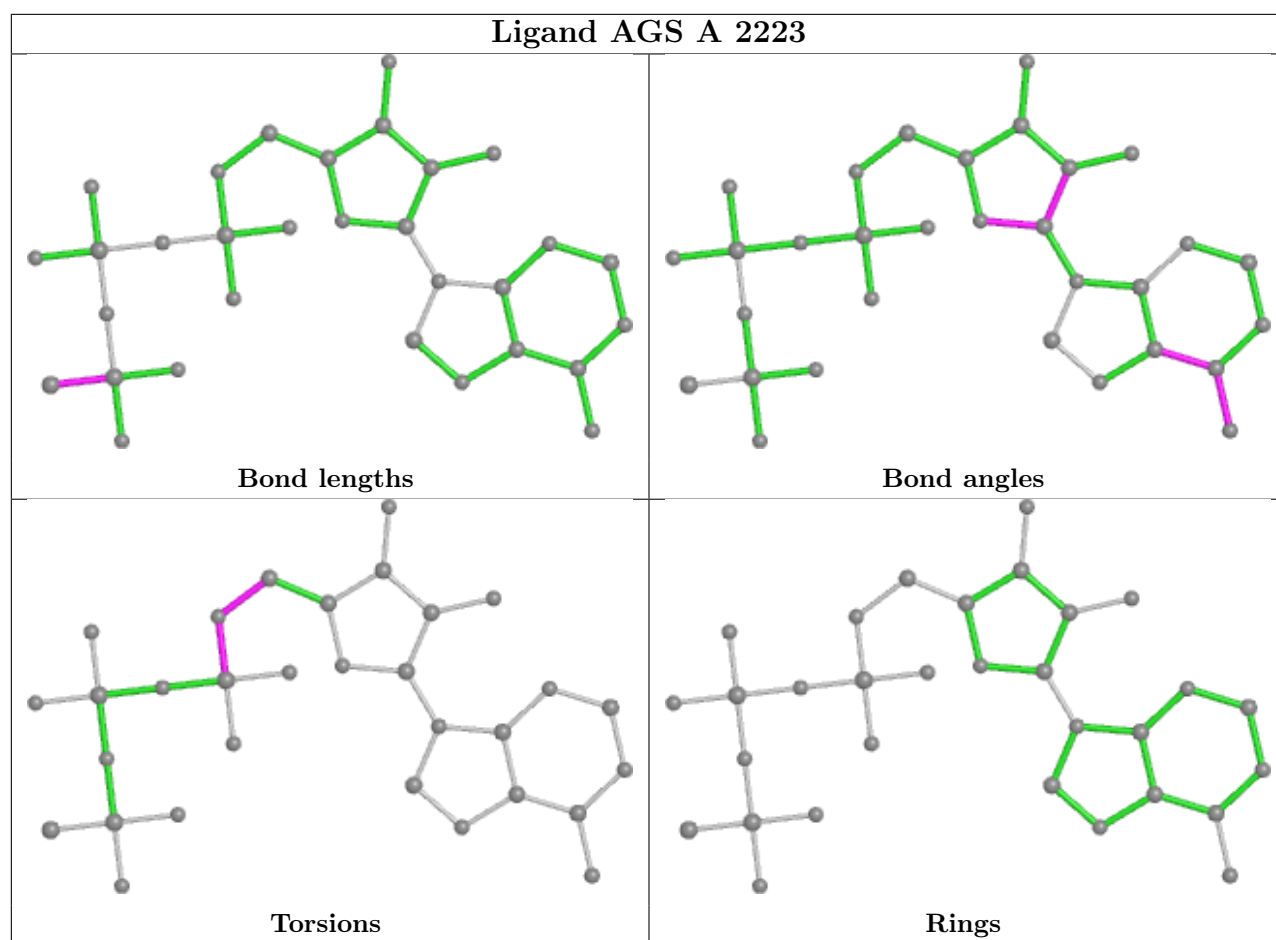
There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2224	AGS	3	0
3	A	2202	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 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.

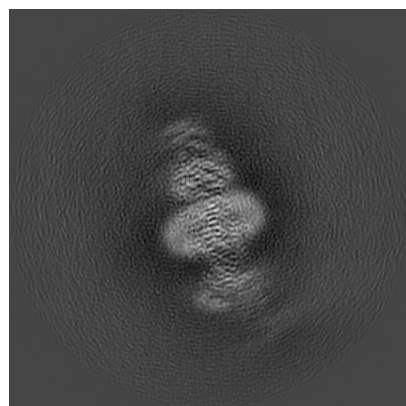
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-28041. These allow visual inspection of the internal detail of the map and identification of artifacts.

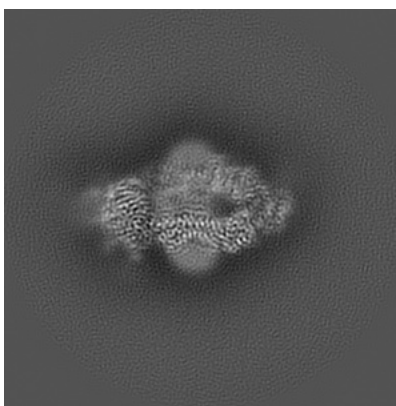
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

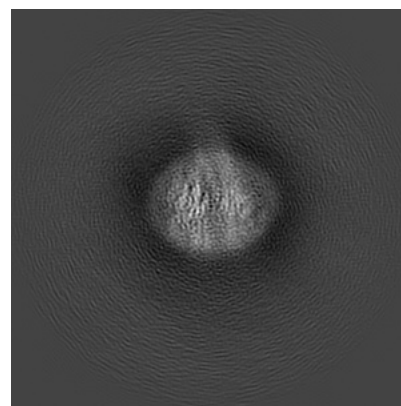
6.1.1 Primary map



X

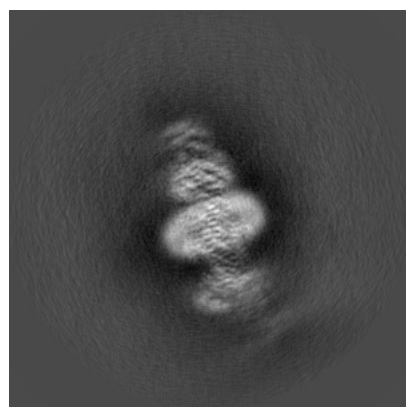


Y

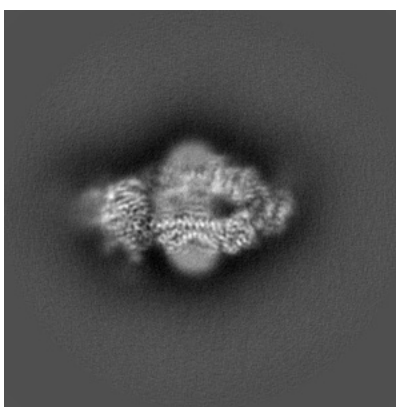


Z

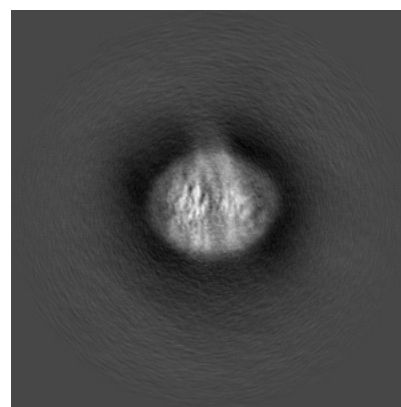
6.1.2 Raw map



X



Y

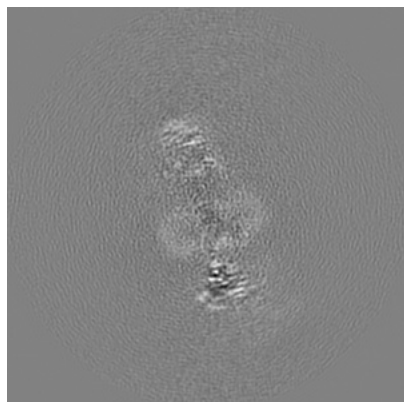


Z

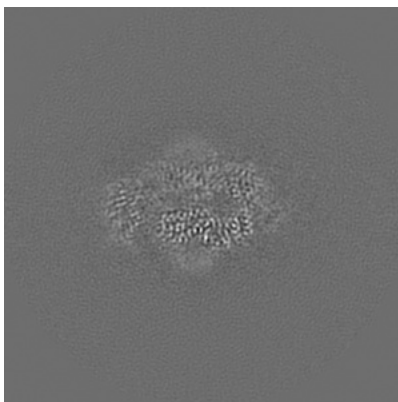
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

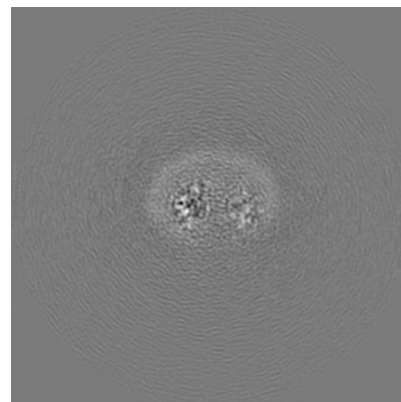
6.2.1 Primary map



X Index: 192

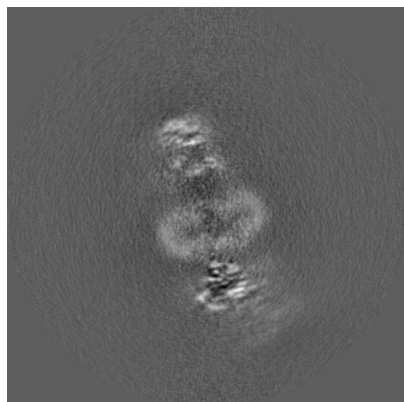


Y Index: 192

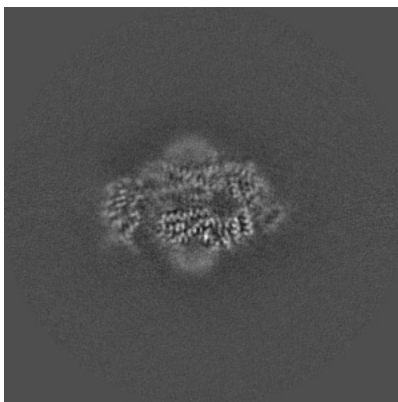


Z Index: 192

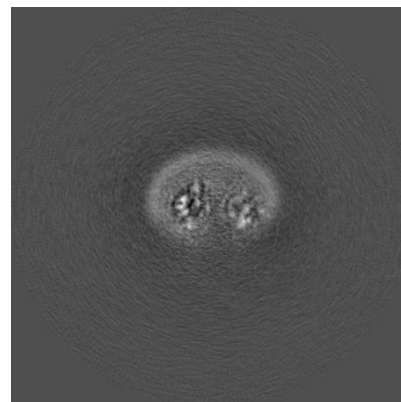
6.2.2 Raw map



X Index: 192



Y Index: 192

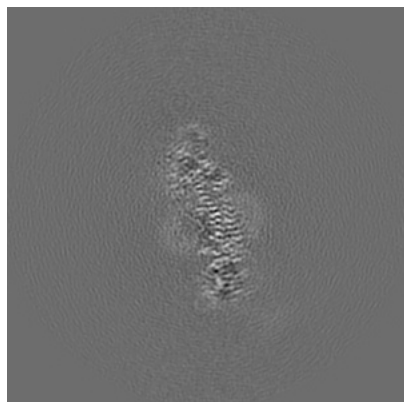


Z Index: 192

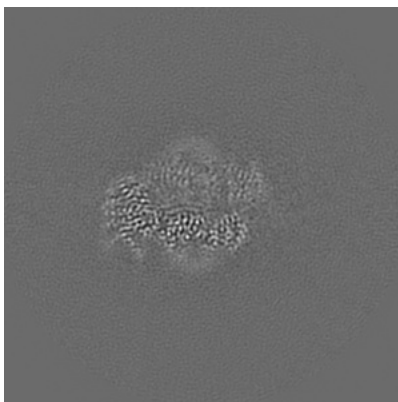
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

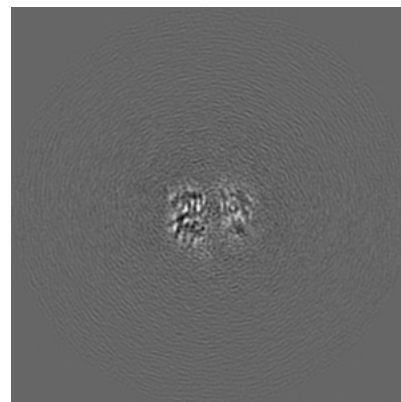
6.3.1 Primary map



X Index: 177

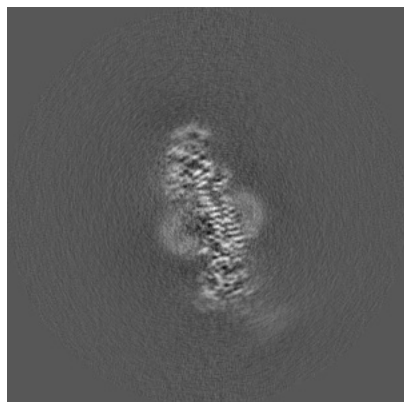


Y Index: 201

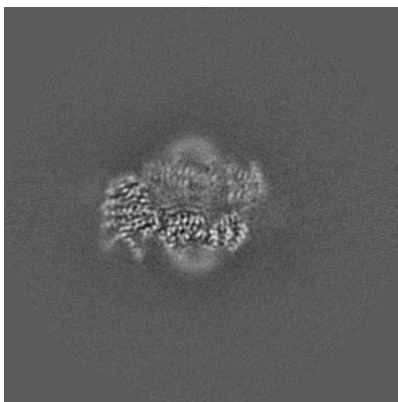


Z Index: 222

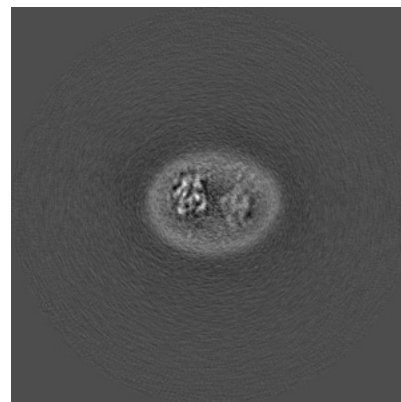
6.3.2 Raw map



X Index: 178



Y Index: 201

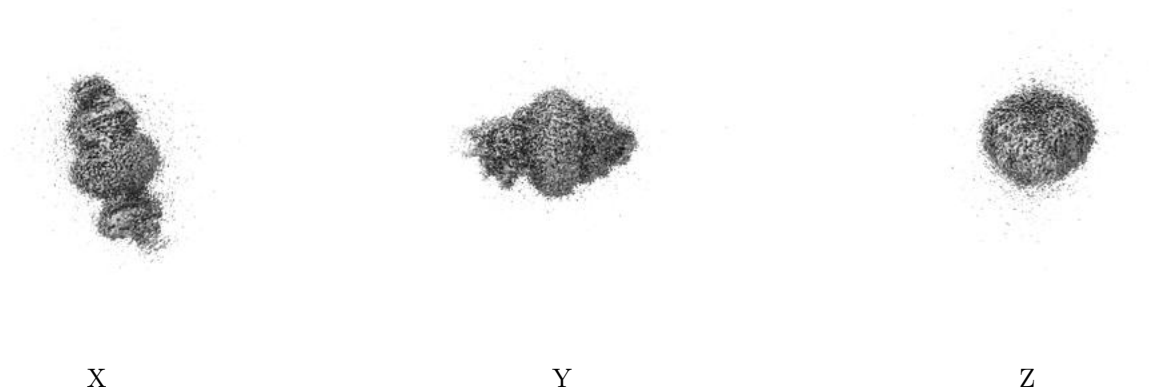


Z Index: 173

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

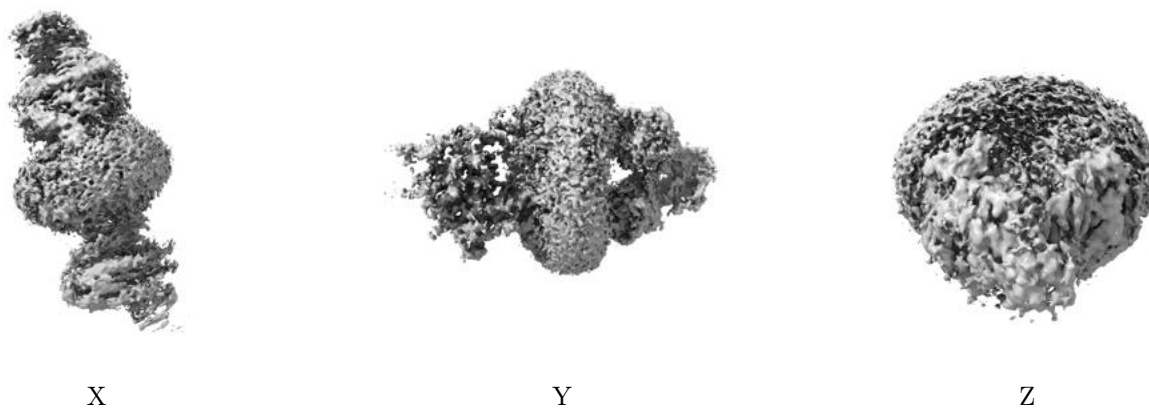
6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.018. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.4.2 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.

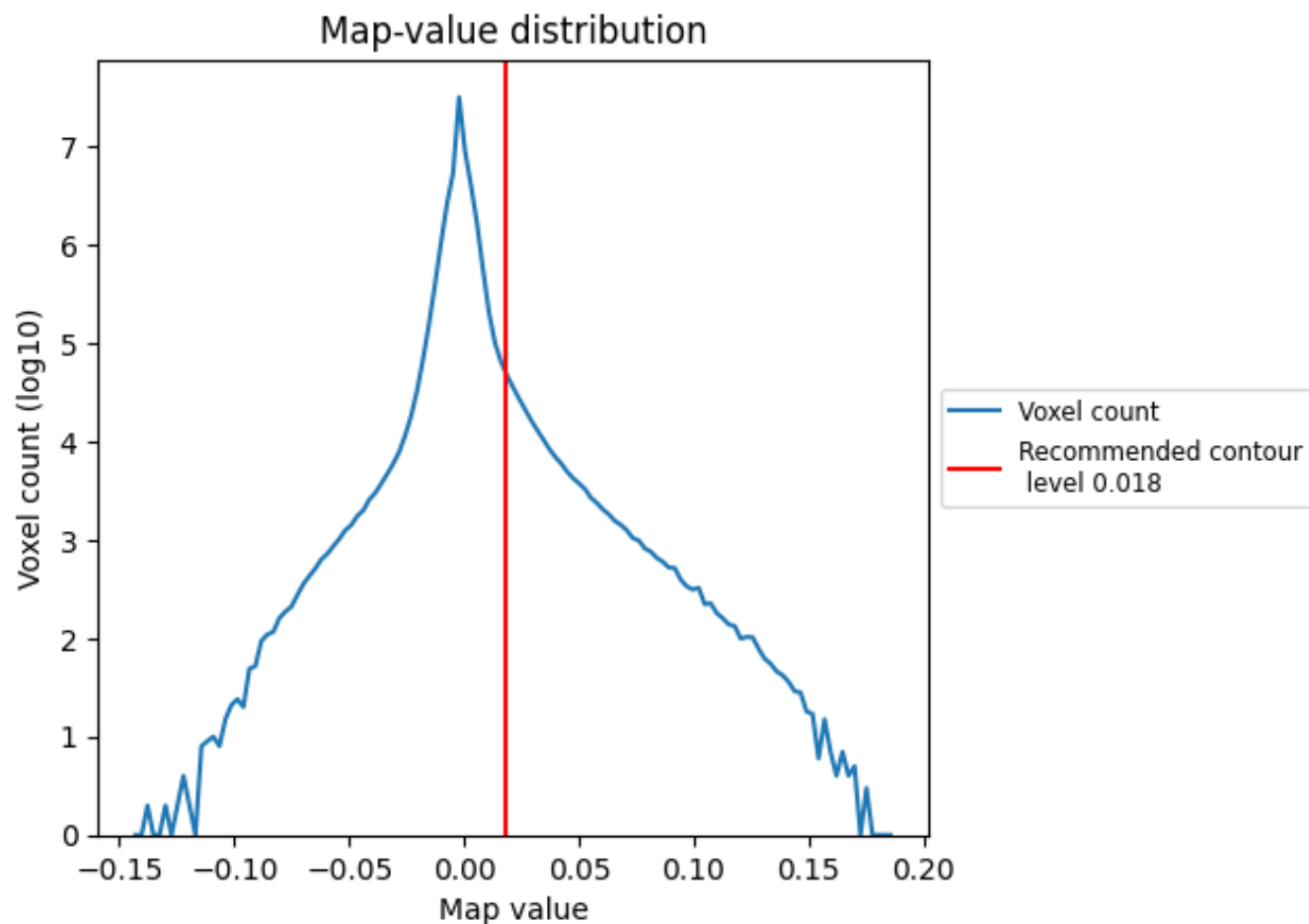
6.5 Mask visualisation [i](#)

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

7 Map analysis [i](#)

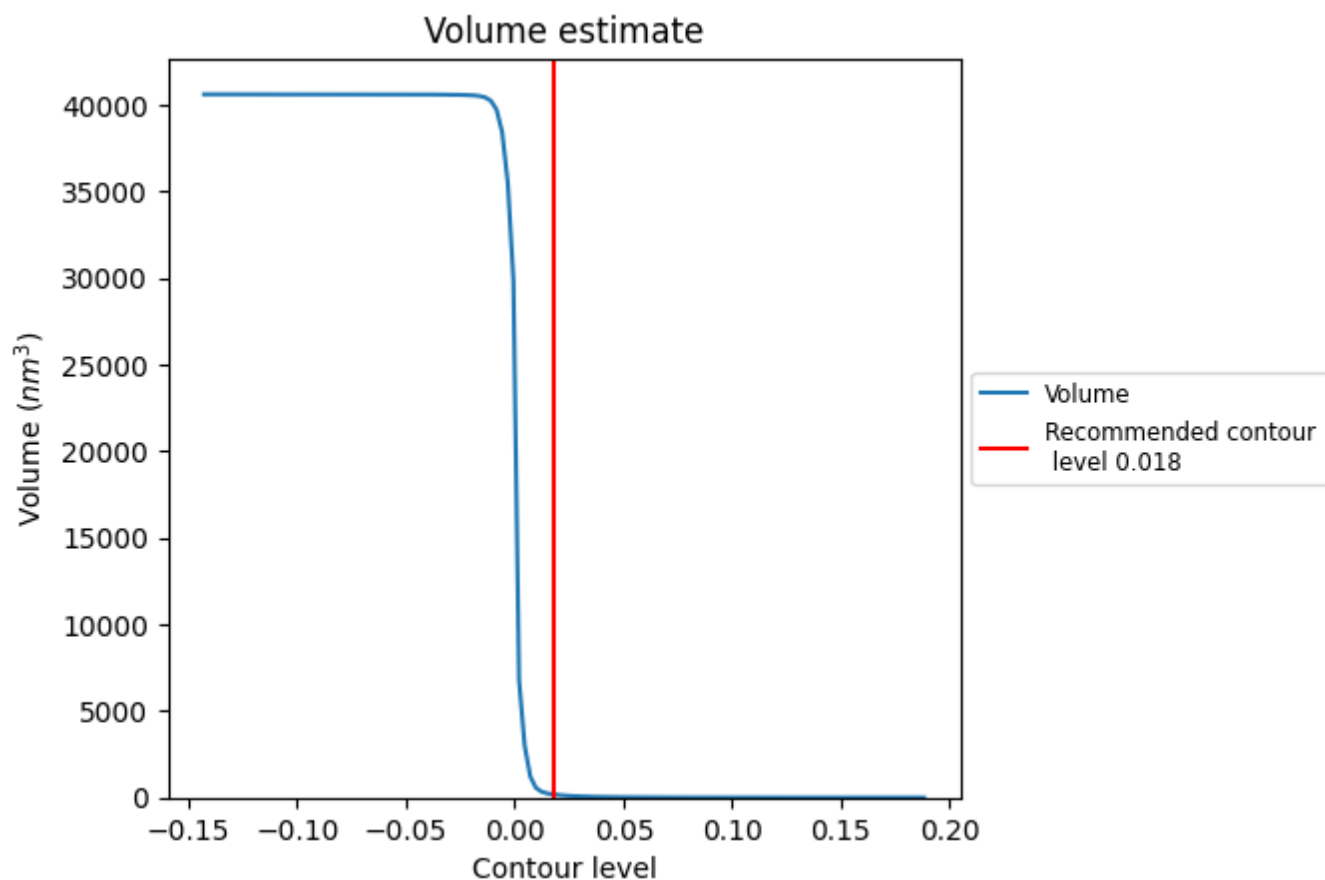
This section contains the results of statistical analysis of the map.

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.

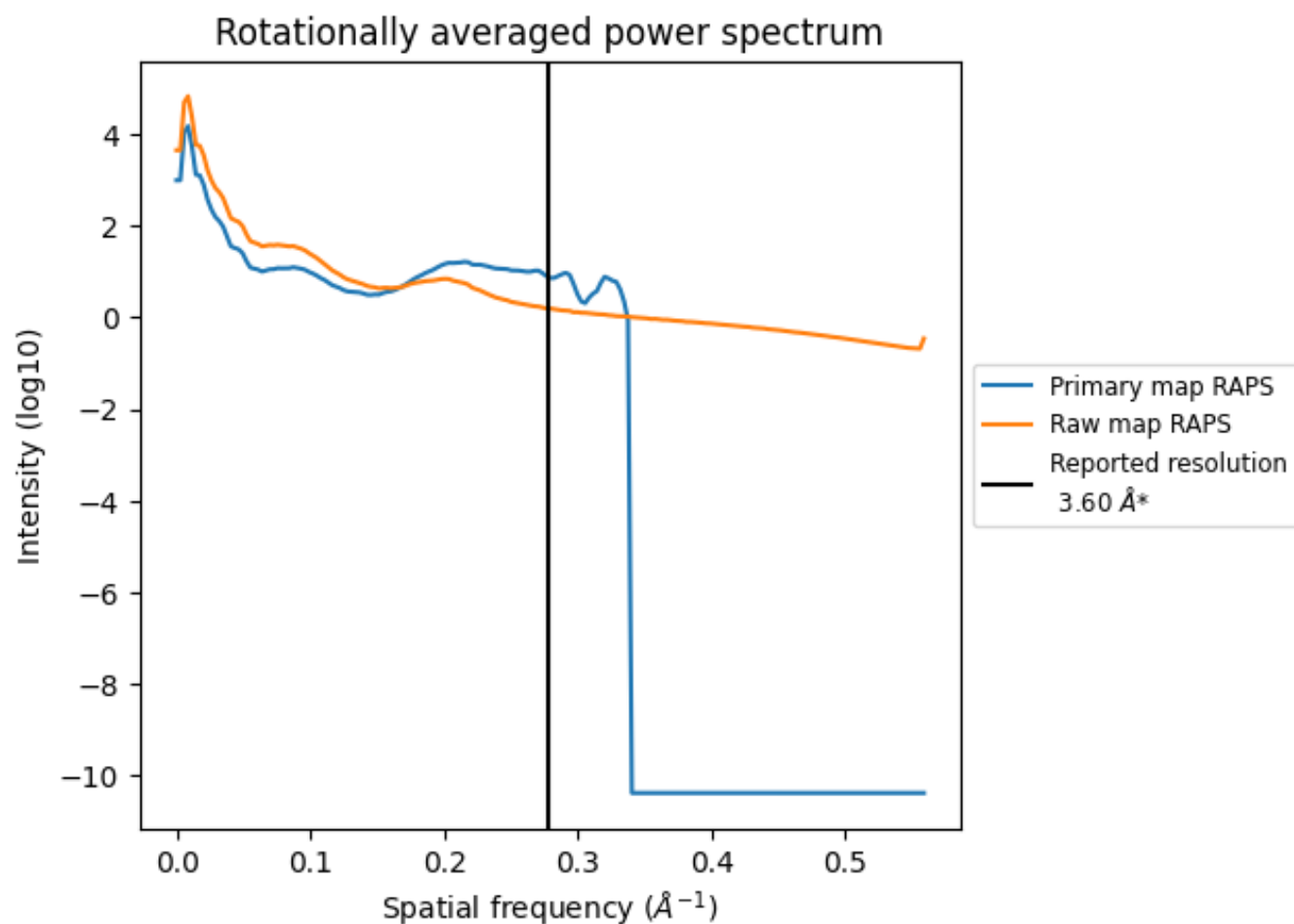
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 178 nm^3 ; this corresponds to an approximate mass of 161 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 ⓘ

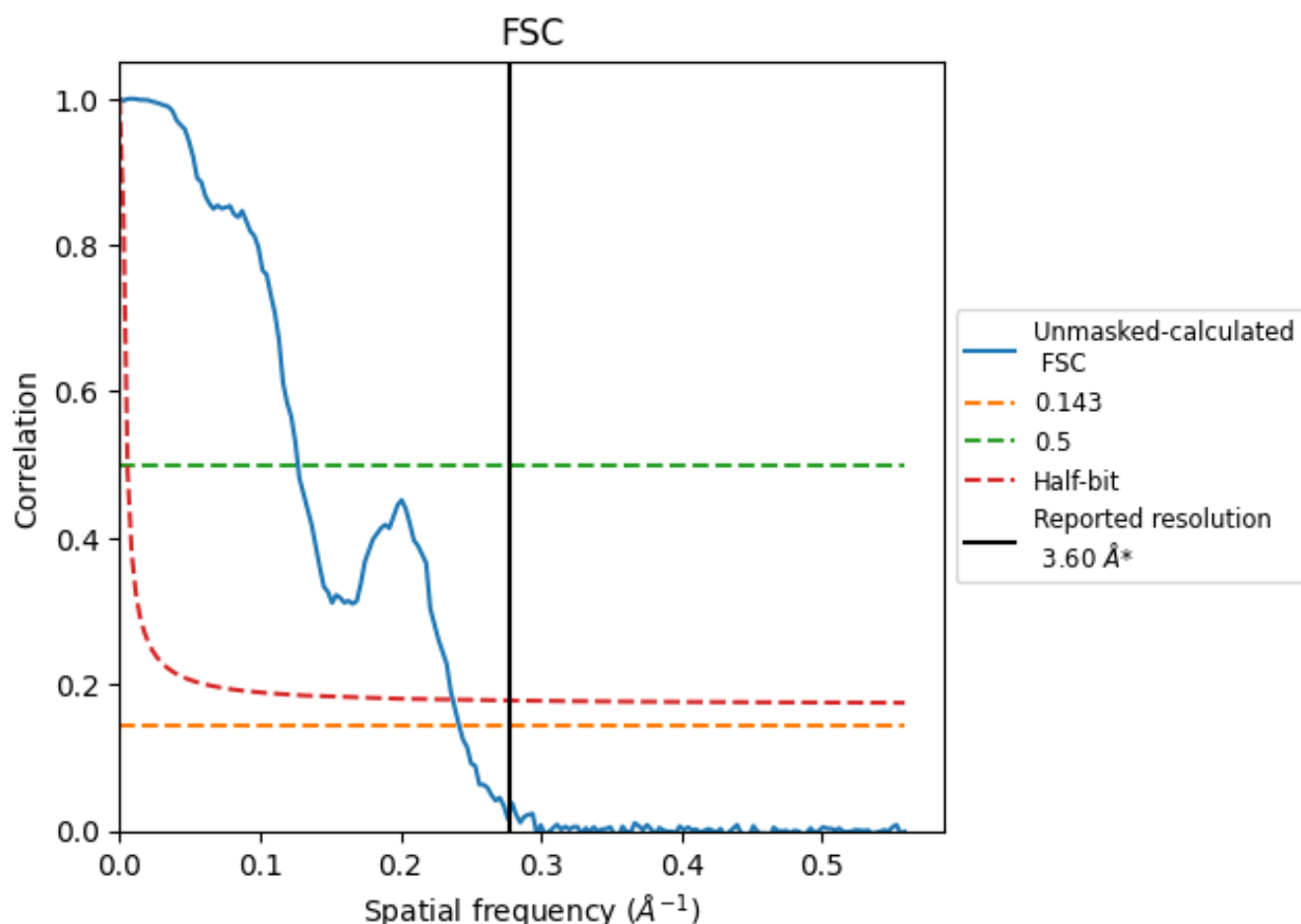


*Reported resolution corresponds to spatial frequency of 0.278 Å⁻¹

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 0.278 Å⁻¹

8.2 Resolution estimates [i](#)

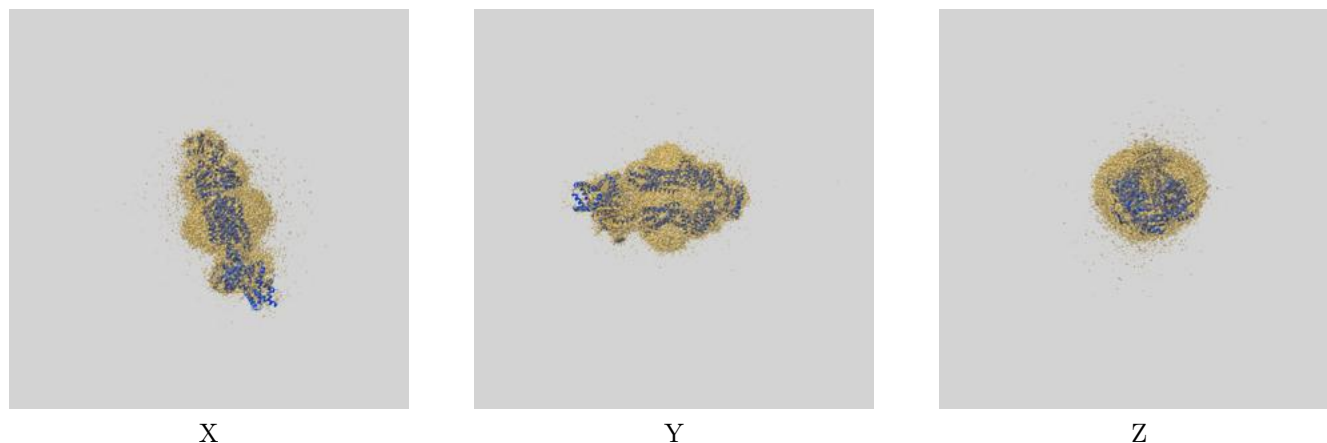
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.14	7.88	4.22

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 4.14 differs from the reported value 3.6 by more than 10 %

9 Map-model fit [i](#)

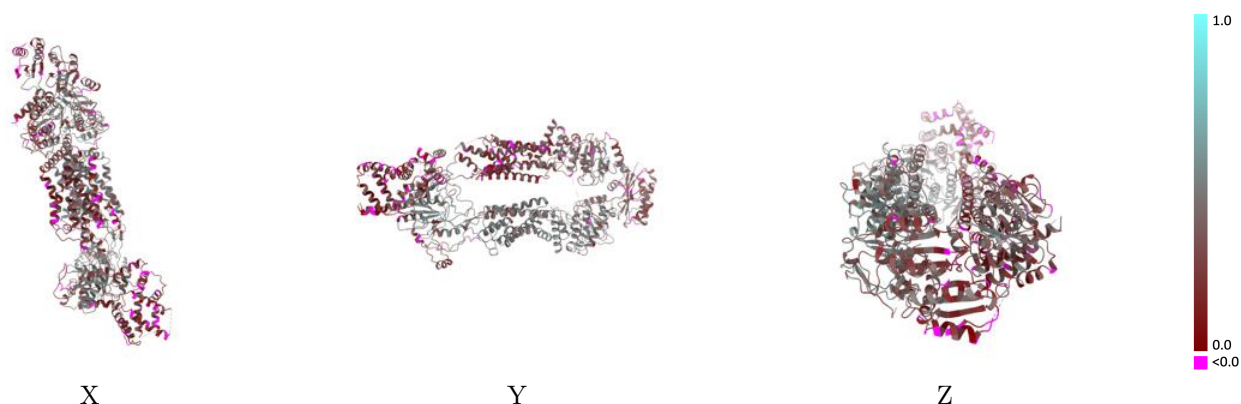
This section contains information regarding the fit between EMDB map EMD-28041 and PDB model 8EDW. Per-residue inclusion information can be found in [section 3](#) on [page 6](#).

9.1 Map-model overlay [i](#)



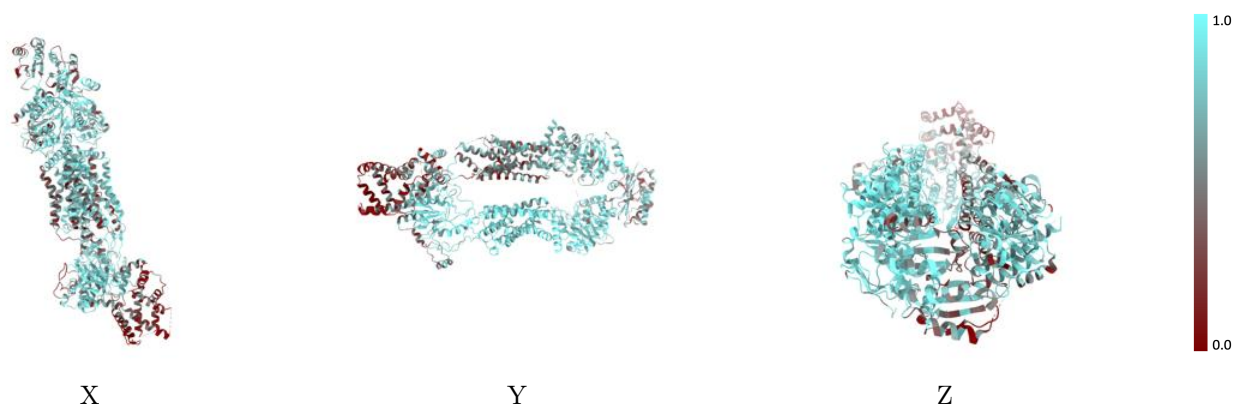
The images above show the 3D surface view of the map at the recommended contour level 0.018 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



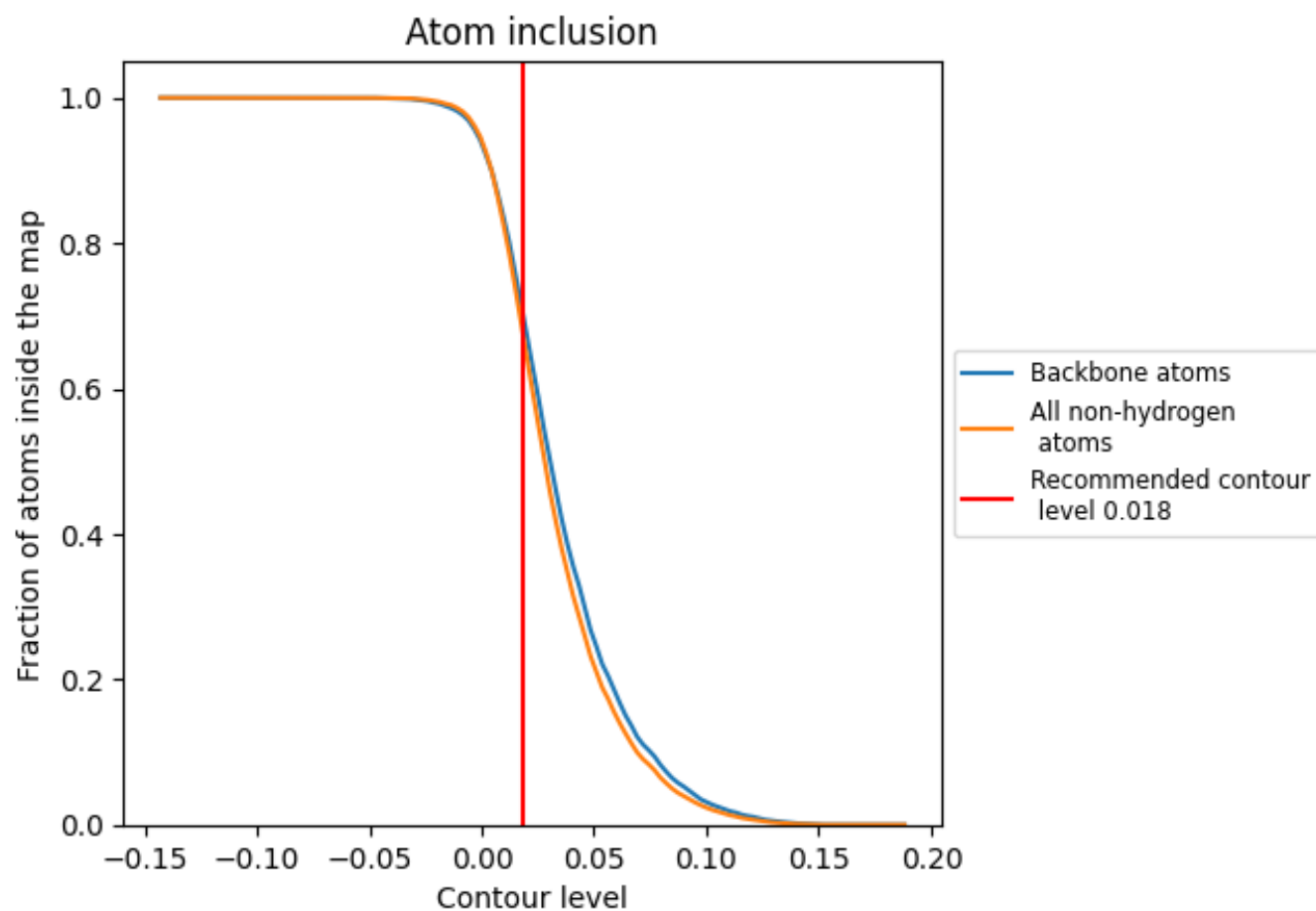
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.018).

9.4 Atom inclusion [i](#)



At the recommended contour level, 71% of all backbone atoms, 68% 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 (0.018) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6814	<div></div> 0.3400
A	<div></div> 0.6814	<div></div> 0.3400
B	<div></div> 0.6786	<div></div> 0.4150
D	<div></div> 0.7143	<div></div> 0.3710

