



Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 10:43 AM UTC

PDB ID : 5XJY / pdb_00005xjy
EMDB ID : EMD-6724
Title : Cryo-EM structure of human ABCA1
Authors : Qian, H.W.; Yan, N.; Gong, X.
Deposited on : 2017-05-04
Resolution : 4.10 Å(reported)

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

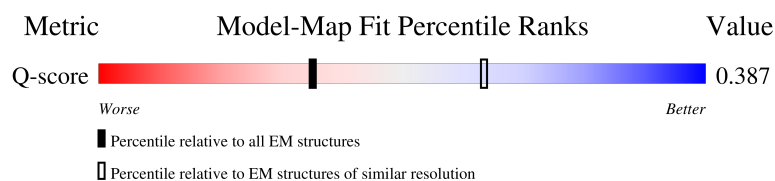
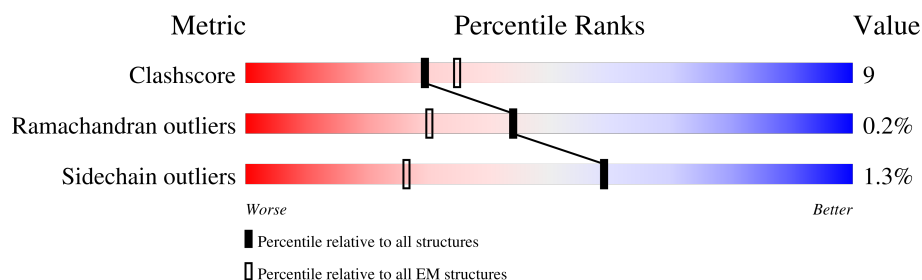
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	6458 (3.60 - 4.60)

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	2305	19% 67% 15% 18%
2	B	5	40% 60%
3	C	2	50% 50%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 12785 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 ATP-binding cassette sub-family A member 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1901	Total	C	N	O	S	0	0
			12626	8005	2236	2328	57		

There are 44 discrepancies between the modelled and reference sequences:

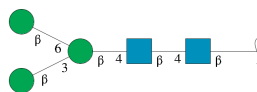
Chain	Residue	Modelled	Actual	Comment	Reference
A	-20	MET	-	expression tag	UNP O95477
A	-19	ALA	-	expression tag	UNP O95477
A	-18	ASP	-	expression tag	UNP O95477
A	-17	TYR	-	expression tag	UNP O95477
A	-16	LYS	-	expression tag	UNP O95477
A	-15	ASP	-	expression tag	UNP O95477
A	-14	ASP	-	expression tag	UNP O95477
A	-13	ASP	-	expression tag	UNP O95477
A	-12	ASP	-	expression tag	UNP O95477
A	-11	LYS	-	expression tag	UNP O95477
A	-10	SER	-	expression tag	UNP O95477
A	-9	GLY	-	expression tag	UNP O95477
A	-8	PRO	-	expression tag	UNP O95477
A	-7	ASP	-	expression tag	UNP O95477
A	-6	GLU	-	expression tag	UNP O95477
A	-5	VAL	-	expression tag	UNP O95477
A	-4	ASP	-	expression tag	UNP O95477
A	-3	ALA	-	expression tag	UNP O95477
A	-2	SER	-	expression tag	UNP O95477
A	-1	GLY	-	expression tag	UNP O95477
A	0	ARG	-	expression tag	UNP O95477
A	2262	LEU	-	expression tag	UNP O95477
A	2263	GLU	-	expression tag	UNP O95477
A	2264	GLY	-	expression tag	UNP O95477
A	2265	SER	-	expression tag	UNP O95477
A	2266	ASP	-	expression tag	UNP O95477
A	2267	GLU	-	expression tag	UNP O95477
A	2268	VAL	-	expression tag	UNP O95477

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Chain	Residue	Modelled	Actual	Comment	Reference
A	2269	ASP	-	expression tag	UNP O95477
A	2270	ALA	-	expression tag	UNP O95477
A	2271	VAL	-	expression tag	UNP O95477
A	2272	GLU	-	expression tag	UNP O95477
A	2273	GLY	-	expression tag	UNP O95477
A	2274	SER	-	expression tag	UNP O95477
A	2275	HIS	-	expression tag	UNP O95477
A	2276	HIS	-	expression tag	UNP O95477
A	2277	HIS	-	expression tag	UNP O95477
A	2278	HIS	-	expression tag	UNP O95477
A	2279	HIS	-	expression tag	UNP O95477
A	2280	HIS	-	expression tag	UNP O95477
A	2281	HIS	-	expression tag	UNP O95477
A	2282	HIS	-	expression tag	UNP O95477
A	2283	HIS	-	expression tag	UNP O95477
A	2284	HIS	-	expression tag	UNP O95477

- Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



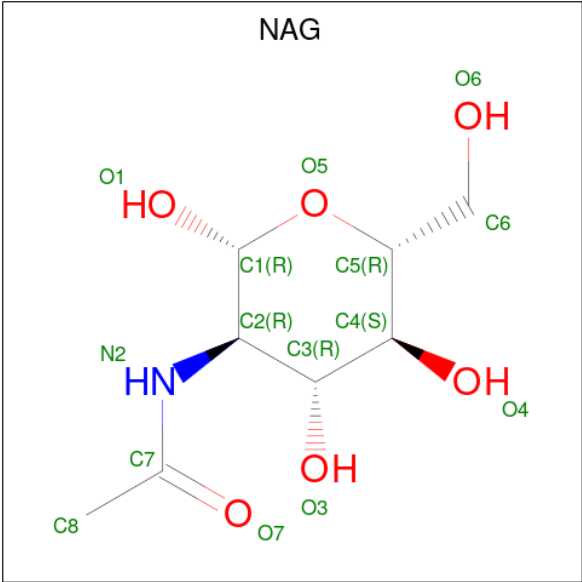
Mol	Chain	Residues	Atoms				AltConf	Trace
2	B	5	Total	C	N	O	0	0
			61	34	2	25		

- Molecule 3 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
3	C	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

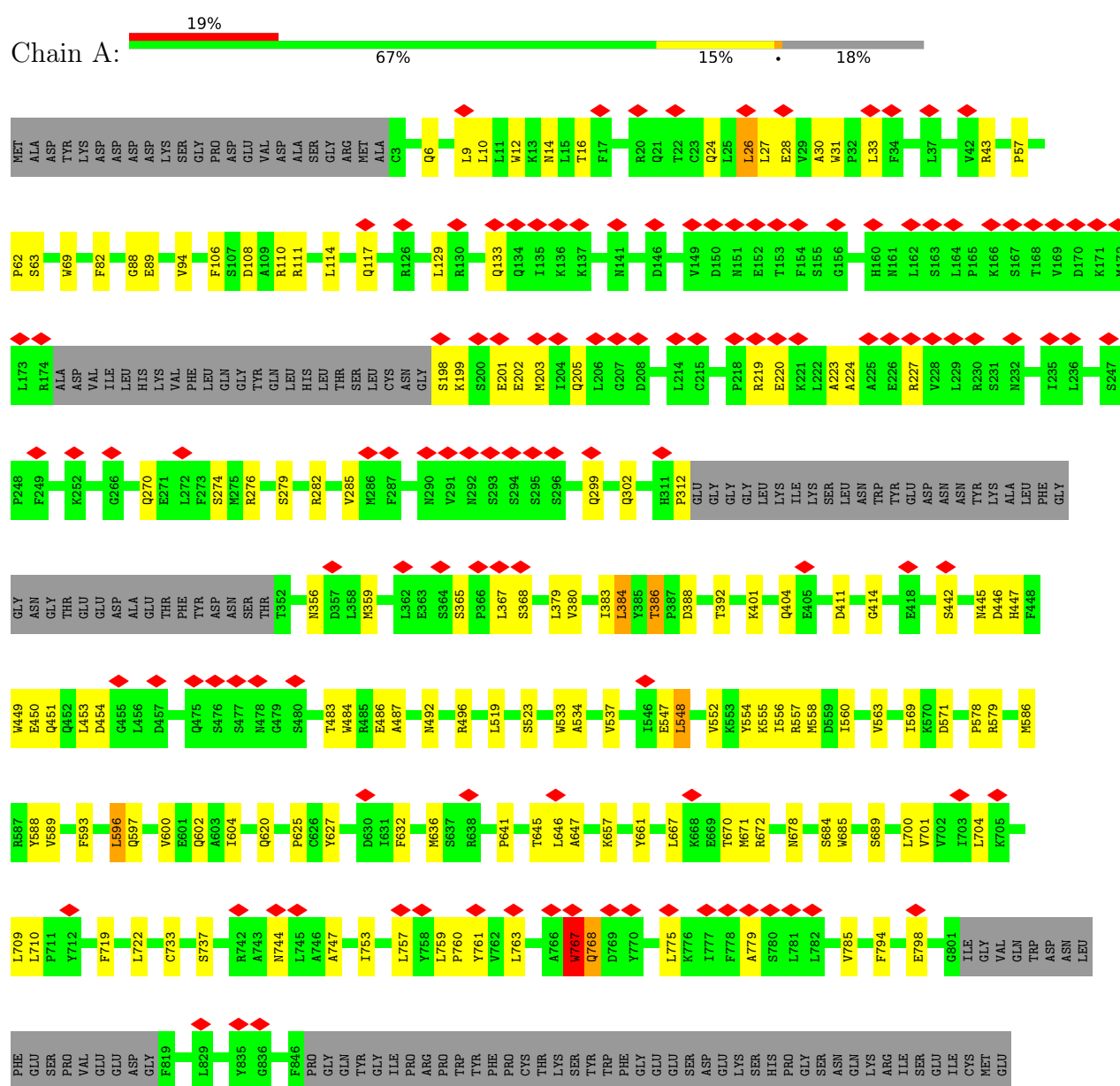


Mol	Chain	Residues	Atoms				AltConf
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	
4	A	1	Total	C	N	O	0
			14	8	1	5	

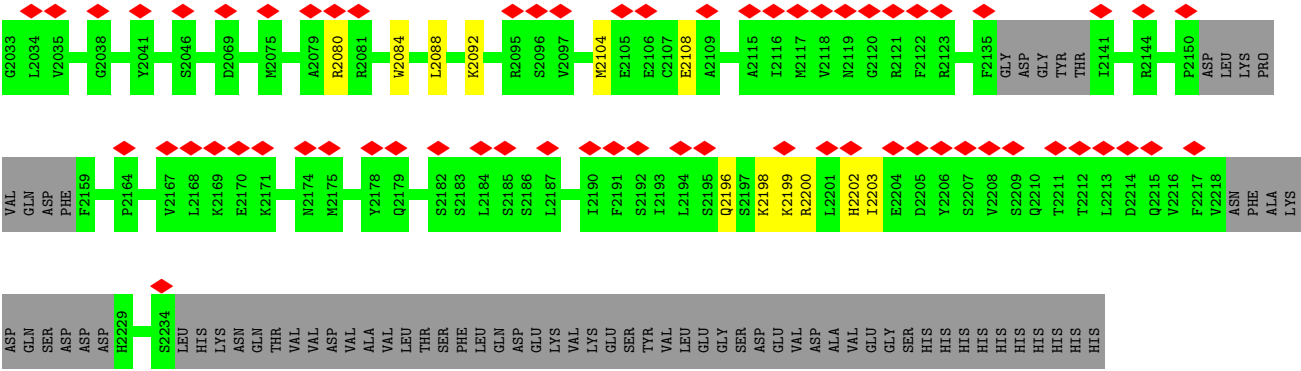
3 Residue-property plots

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.

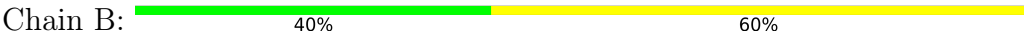
- Molecule 1: ATP-binding cassette sub-family A member 1



T1960	G1961	D1962	T1963	T1964	V1965	T1966	G1967	G1968	D1969	A1970	F1971	L1972	N1973	K1974	S1975	S1976	I1977	L1978	S1979	N1980	I1981	H1982	E1983	V1984	H1985	Q1986	N1987	N1988	G1989	Q1993	A1996	I1997	T1998	T2002	E2005	H2006	F2009	G2015	V2016	P2017	E2020	V2021	G2022	K2023	G2025	E2026	I2029	R2030	K2031	L2032											
GLN	ARG	ILE	LEU	ASP	GLY	GLY	GLN	ASN	ASP	ILE	GLU	ILE	LYS	E1916	L1917	T1918	K1919	I1920	Y1921	R1922	ARG	LYS	ARG	ARG	PRO	ALA	VAL	ASP	ARG	ILE	C1933	V1934	G1935	I1936	F1937	G1938	E1939	C1941	F1942	G1943	L1944	L1945	G1946	V1947	N1948	G1949	A1950	G1951	K1952	S1953	S1954	T1955	F1956	K1957	M1958	L1959					
R1817	G1818	L1819	I1820	D1821	M1822	M1828	L1832	F1835	G1836	F1840	V1841	S1842	L1853	F1854	A1855	M1856	A1857	V1858	E1859	G1860	V1861	V1862	F1863	I1866	T1867	I1870	F1875	ILE	ARG	PRO	ARG	PRO	VAL	ASN	ALA	LYS	L1796	N1797	N1798	I1799	N1800	L1803	K1804	F1807	L1808	I1809	F1810	P1811	H1812	F1813	C1814	L1815	G1816								
L1740	L1741	L1744	Y1745	I1749	Y1754	P1755	A1756	K1761	A1766	Y1767	L1770	V1773	N1774	L1775	F1776	I1779	N1780	G1781	S1782	V1783	A1784	T1785	F1786	V1787	L1788	E1789	LEU	PHE	THR	ASN	ASP	LYS	L1796	N1797	N1798	I1799	N1800	L1803	K1804	F1807	L1808	I1809	F1810	P1811	H1812	F1813	C1814	L1815	G1816												
D1654	V1655	L1656	V1657	S1658	T1659	C1660	V1661	F1663	A1664	M1665	S1666	A1670	Q1678	E1679	R1680	K1683	A1684	K1685	H1686	L1687	Q1688	F1689	I1690	S1691	G1692	I1697	S1701	W1705	D1706	A1714	T1715	L1716	V1717	I1718	I1719	I1720	F1721	G1723	F1724	Q1725	Q1726	K1727	S1728	V1729	V1730	S1731	N1734														
V1551	A1554	I1555	K1556	Q1557	M1558	K1559	L1564	A1565	S1568	D1571	R1572	N1575	M1581	V1590	V1592	N1596	W1599	S1603	N1607	V1608	I1609	M1610	M1611	I1612	I1613	E1622	N1623	P1624	S1625	H1626	T1630	A1631	F1632	N1633	H1634	F1635	L1636	N1637	T1638	Q1639	K1640	Q1641	Q1642	M1649																	
M1446	D1447	L1448	F1449	Q1450	N1451	G1452	N1453	W1454	M1455	Q1457	P1459	S1460	P1461	C1465	K1469	I1470	L1474	C1477	A1481	G1482	G1483	L1484	K1490	Q1491	N1492	I1496	D1507	V1510	K1511	K1522	N1523	K1524	I1525	W1526	F1535	N1541	T1542	Q1543	A1544	L1545	P1546	F1547	S1548	Q1549	E1550																
W1322	K1335	R1336	R1341	R1342	S1343	R1344	K1345	G1346	V1358	G1359	I1360	F1364	V1368	P1369	P1370	K1373	L1379	Q1380	P1381	M1382	M1383	Y1384	N1385	Y1388	V1391	E1397	D1398	L1402	L1405	N1406	G1415	T1416	R1417	C1418	T1424	P1425	D1426	T1427	A1431	E1434	A1439																				
SER	ASP	GLY	THR	LEU	PRO	ALA	ARG	ARG	ASN	ARG	ALA	PHE	GLY	ASP	LYS	CYS	LEU	ARG	PRO	PHE	THR	GLU	ASP	ASP	ALA	ALA	ASP	ASN	ASP	SER	ILE	ASP	ILE	THR	LEU	GLY	LEU	GLY	ILE	PHE	LEU	LYS	VAL	ALA	GLU	GLY	SER	GLY	VAL	GLY	THR										
I1200	G1201	H1202	E1203	L1204	T1205	Y1206	L1207	L1208	P1209	Y1210	E1211	A1212	A1213	K1214	E1215	G1216	A1217	L1221	F1222	H1223	GLU	ILE	ASP	ASP	PRO	ASN	ARG	LEU	SER	D1231	L1232	G1233	I1234	S1235	S1236	Y1237	G1238	ILE	SER	GLU	THR	THR	GLY	MET	ASP	GLY	ILE	PHE	LEU	LYS	VAL	ALA	GLU	GLY	SER	GLY	VAL	ASP	ALA	GLU	THR
Q1121	L1122	GLY	THR	GLY	TYR	TYR	L1128	T1129	L1139	S1140	S1141	C1142	R1143	S1146	Y1151	LEU	LYS	GLU	ASP	SER	VAL	GLN	SER	SER	SER	SER	D1164	D1170	H1171	E1172	S1173	D1174	T1175	L1176	T1177	I1178	D1179	V1180	S1181	A1182	I1183	S1184	I1187	H1190	E1193	A1194	R1195	L1196	V1197	E1198	D1199										
D963	L964	R965	S966	E967	M968	S969		Q973	L984	F985	F996	L1000		S1004		G1020		S1023	S1024	K1025	L1026	K1027	S1028		G1035	K1040	A1044		G1050	S1051		S1067	R1068	R1069		W1072	E1073		L1076		D1095		P951	P952	T953	S954	G955	T956	A957	Y958	I959	L960	G961	K962							



● Molecule 2: beta-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	790156	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.485	Depositor
Minimum map value	-0.354	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.011	Depositor
Recommended contour level	0.06	Depositor
Map size (Å)	261.308, 261.308, 261.308	wwPDB
Map dimensions	200, 200, 200	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.30654, 1.30654, 1.30654	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	0.43	0/12840	0.76	9/17577 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	15

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	926	GLY	CA-C-N	6.41	133.77	121.54
1	A	926	GLY	C-N-CA	6.41	133.77	121.54
1	A	768	GLN	N-CA-CB	-6.11	107.20	114.17
1	A	759	LEU	N-CA-C	5.74	122.50	109.81
1	A	1382	TRP	CA-C-N	5.37	131.79	121.54
1	A	1382	TRP	C-N-CA	5.37	131.79	121.54
1	A	1636	LEU	CA-CB-CG	5.25	134.69	116.30
1	A	767	TRP	CA-C-N	-5.05	117.51	126.45
1	A	767	TRP	C-N-CA	-5.05	117.51	126.45

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1427	THR	Peptide

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Mol	Chain	Res	Type	Group
1	A	1458	ASN	Peptide
1	A	1460	SER	Peptide
1	A	1474	LEU	Peptide
1	A	1483	GLY	Peptide
1	A	1546	PRO	Peptide
1	A	1721	PHE	Peptide
1	A	1998	THR	Peptide
1	A	384	LEU	Peptide
1	A	386	THR	Peptide
1	A	586	MET	Peptide
1	A	589	VAL	Peptide
1	A	927	GLN	Peptide
1	A	94	VAL	Peptide
1	A	985	PHE	Peptide

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	12626	0	10430	215	0
2	B	61	0	52	0	0
3	C	28	0	25	0	0
4	A	70	0	65	0	0
All	All	12785	0	10572	215	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 9.

All (215) 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:1817:ARG:O	1:A:1821:ASP:HB2	1.80	0.81
1:A:1816:GLY:O	1:A:1820:ILE:HB	1.83	0.79
1:A:1402:LEU:O	1:A:1406:ASN:HB2	1.86	0.76
1:A:1685:LYS:O	1:A:1689:PHE:HB2	1.86	0.75
1:A:1461:PRO:HB3	1:A:1483:GLY:H	1.53	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:767:TRP:O	1:A:768:GLN:HB3	1.89	0.72
1:A:794:PHE:O	1:A:798:GLU:HB2	1.92	0.69
1:A:1592:VAL:HG22	1:A:1609:ILE:HD12	1.74	0.69
1:A:700:LEU:O	1:A:704:LEU:HB2	1.94	0.68
1:A:700:LEU:HD12	1:A:722:LEU:HD11	1.76	0.67
1:A:1658:SER:HB2	1:A:1822:MET:HE3	1.80	0.64
1:A:1662:ILE:O	1:A:1666:SER:CB	2.47	0.63
1:A:1418:CYS:HB2	1:A:1626:HIS:HA	1.81	0.62
1:A:571:ASP:HA	1:A:1599:TRP:HE1	1.63	0.62
1:A:733:CYS:O	1:A:737:SER:HB2	2.00	0.61
1:A:1183:ILE:HA	1:A:1196:LEU:HA	1.81	0.61
1:A:1741:LEU:O	1:A:1745:TYR:HB2	2.01	0.60
1:A:625:PRO:HB3	1:A:1510:VAL:HG13	1.82	0.60
1:A:1069:ARG:O	1:A:1073:GLU:CB	2.50	0.60
1:A:1828:MET:O	1:A:1832:LEU:HB2	2.02	0.60
1:A:12:TRP:O	1:A:16:THR:OG1	2.21	0.59
1:A:270:GLN:O	1:A:274:SER:HB3	2.02	0.59
1:A:1680:ARG:HH22	1:A:1761:LYS:HE2	1.68	0.59
1:A:379:LEU:HD12	1:A:380:VAL:HG23	1.83	0.59
1:A:1391:VAL:HG11	1:A:1405:LEU:HD13	1.85	0.59
1:A:6:GLN:O	1:A:10:LEU:HB2	2.03	0.59
1:A:14:ASN:ND2	1:A:684:SER:OG	2.35	0.59
1:A:557:ARG:HH21	1:A:1634:HIS:CE1	2.20	0.59
1:A:1465:CYS:SG	1:A:1477:CYS:N	2.75	0.59
1:A:26:LEU:O	1:A:30:ALA:HB3	2.03	0.58
1:A:31:TRP:HD1	1:A:647:ALA:HA	1.68	0.58
1:A:1766:ALA:O	1:A:1770:LEU:HB2	2.02	0.58
1:A:89:GLU:OE2	1:A:620:GLN:NE2	2.37	0.58
1:A:1424:ILE:HG13	1:A:1425:PRO:HD3	1.84	0.58
1:A:1731:SER:OG	1:A:1734:ASN:ND2	2.36	0.58
1:A:106:PHE:HB3	1:A:1581:MET:HE1	1.84	0.58
1:A:446:ASP:O	1:A:450:GLU:CB	2.52	0.58
1:A:1683:LYS:O	1:A:1687:LEU:CB	2.51	0.58
1:A:519:LEU:O	1:A:523:SER:HB2	2.04	0.57
1:A:1685:LYS:O	1:A:1689:PHE:CB	2.51	0.57
1:A:767:TRP:O	1:A:768:GLN:CB	2.52	0.57
1:A:2196:GLN:O	1:A:2200:ARG:CB	2.53	0.57
1:A:1448:LEU:HB2	1:A:1484:LEU:HD11	1.87	0.56
1:A:1198:GLU:O	1:A:1231:ASP:N	2.39	0.55
1:A:1415:GLY:O	1:A:1611:ASN:ND2	2.39	0.55
1:A:1855:ALA:O	1:A:1859:GLU:CB	2.54	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:LEU:HD21	1:A:996:PHE:HA	1.87	0.55
1:A:447:HIS:O	1:A:451:GLN:CB	2.53	0.55
1:A:1727:LYS:NZ	1:A:1821:ASP:OD2	2.35	0.55
1:A:1456:MET:O	1:A:1460:SER:OG	2.23	0.55
1:A:2017:PRO:O	1:A:2021:VAL:N	2.37	0.54
1:A:88:GLY:O	1:A:1591:LYS:NZ	2.37	0.54
1:A:1684:ALA:HA	1:A:1687:LEU:HB3	1.88	0.54
1:A:1068:ARG:O	1:A:1072:TRP:CB	2.56	0.54
1:A:1662:ILE:O	1:A:1666:SER:HB2	2.08	0.54
1:A:1684:ALA:O	1:A:1688:GLN:HB2	2.07	0.54
1:A:1447:ASP:O	1:A:1451:ASN:ND2	2.41	0.54
1:A:537:VAL:HB	1:A:555:LYS:HB3	1.90	0.54
1:A:1800:ASN:O	1:A:1804:LYS:CB	2.56	0.54
1:A:641:PRO:O	1:A:645:THR:OG1	2.23	0.54
1:A:282:ARG:HA	1:A:285:VAL:HG22	1.91	0.53
1:A:1524:LYS:HZ1	1:A:1526:TRP:HD1	1.57	0.53
1:A:1809:ILE:HA	1:A:1812:HIS:HB3	1.90	0.53
1:A:554:TYR:HE2	1:A:556:ILE:HD11	1.74	0.53
1:A:632:PHE:O	1:A:636:MET:HB2	2.08	0.53
1:A:1623:ASN:ND2	1:A:1625:SER:OG	2.41	0.53
1:A:1799:ILE:O	1:A:1803:LEU:CB	2.57	0.53
1:A:114:LEU:HD11	1:A:1551:VAL:HG22	1.90	0.53
1:A:1662:ILE:O	1:A:1666:SER:HB3	2.09	0.52
1:A:1417:ARG:HH21	1:A:1417:ARG:H	1.57	0.52
1:A:450:GLU:O	1:A:454:ASP:CB	2.58	0.52
1:A:1683:LYS:O	1:A:1687:LEU:HB2	2.10	0.52
1:A:657:LYS:O	1:A:661:TYR:HB2	2.09	0.52
1:A:108:ASP:OD1	1:A:111:ARG:NH2	2.38	0.51
1:A:483:THR:HG23	1:A:486:GLU:H	1.75	0.51
1:A:1343:SER:HB2	1:A:1346:GLY:HA3	1.92	0.51
1:A:1571:ASP:OD1	1:A:1575:ASN:ND2	2.43	0.51
1:A:632:PHE:O	1:A:636:MET:CB	2.57	0.51
1:A:220:GLU:O	1:A:224:ALA:HB2	2.11	0.51
1:A:1490:LYS:NZ	1:A:1492:ASN:OD1	2.39	0.51
1:A:1607:ASN:HD21	1:A:1630:THR:HA	1.75	0.51
1:A:2104:MET:O	1:A:2108:GLU:CB	2.59	0.51
1:A:701:VAL:HG21	1:A:719:PHE:HB2	1.92	0.51
1:A:201:GLU:O	1:A:205:GLN:CB	2.60	0.50
1:A:996:PHE:O	1:A:1000:LEU:CB	2.59	0.50
1:A:1417:ARG:NH1	1:A:1426:ASP:OD2	2.44	0.50
1:A:767:TRP:CE3	1:A:767:TRP:HA	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1683:LYS:O	1:A:1687:LEU:HB3	2.11	0.50
1:A:704:LEU:HD21	1:A:710:LEU:HD12	1.93	0.50
1:A:2088:LEU:O	1:A:2092:LYS:CB	2.59	0.50
1:A:129:LEU:O	1:A:133:GLN:N	2.44	0.50
1:A:563:VAL:HG22	1:A:593:PHE:HB2	1.94	0.50
1:A:519:LEU:O	1:A:523:SER:CB	2.60	0.50
1:A:1388:TYR:HB3	1:A:1496:ILE:H	1.77	0.50
1:A:1670:ALA:HB1	1:A:1767:TYR:HA	1.94	0.49
1:A:1785:THR:HG23	1:A:1819:LEU:HD13	1.93	0.49
1:A:2026:GLU:O	1:A:2030:ARG:CB	2.61	0.49
1:A:760:PRO:HA	1:A:763:LEU:HB2	1.93	0.49
1:A:1719:ILE:HA	1:A:1722:ILE:HG22	1.93	0.49
1:A:1173:SER:O	1:A:1177:THR:CB	2.61	0.49
1:A:220:GLU:O	1:A:224:ALA:CB	2.60	0.49
1:A:1740:LEU:O	1:A:1744:LEU:HB3	2.12	0.49
1:A:2199:LYS:O	1:A:2203:ILE:CB	2.61	0.49
1:A:1655:VAL:HG22	1:A:1822:MET:HG3	1.95	0.49
1:A:1639:THR:OG1	1:A:1640:LYS:N	2.45	0.49
1:A:775:LEU:O	1:A:779:ALA:CB	2.61	0.48
1:A:1507:ASP:OD1	1:A:1511:LYS:NZ	2.41	0.48
1:A:969:SER:O	1:A:973:GLN:CB	2.62	0.48
1:A:1918:THR:HA	1:A:1936:ILE:H	1.78	0.48
1:A:775:LEU:O	1:A:779:ALA:HB2	2.14	0.48
1:A:1717:VAL:HA	1:A:1720:ILE:HD12	1.95	0.48
1:A:12:TRP:O	1:A:16:THR:CB	2.62	0.47
1:A:31:TRP:HE1	1:A:646:LEU:HG	1.79	0.47
1:A:906:LYS:HA	1:A:961:GLY:HA3	1.96	0.47
1:A:547:GLU:HG2	1:A:548:LEU:H	1.78	0.47
1:A:30:ALA:HA	1:A:33:LEU:HD12	1.97	0.47
1:A:117:GLN:O	1:A:1557:GLN:NE2	2.48	0.47
1:A:761:TYR:HB2	1:A:785:VAL:HG12	1.94	0.47
1:A:114:LEU:HD22	1:A:1545:LEU:HB3	1.96	0.47
1:A:1683:LYS:HD2	1:A:1684:ALA:HB2	1.96	0.47
1:A:1955:THR:O	1:A:1959:LEU:CB	2.63	0.47
1:A:24:GLN:O	1:A:28:GLU:HB2	2.15	0.47
1:A:484:TRP:HA	1:A:487:ALA:HB3	1.96	0.47
1:A:1117:PHE:O	1:A:1121:GLN:CB	2.63	0.47
1:A:2002:THR:O	1:A:2006:HIS:CB	2.63	0.47
1:A:442:SER:O	1:A:446:ASP:N	2.47	0.47
1:A:1919:LYS:N	1:A:1934:VAL:O	2.47	0.47
1:A:62:PRO:HG3	1:A:69:TRP:CE2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:199:LYS:O	1:A:203:MET:CB	2.62	0.46
1:A:31:TRP:CD1	1:A:647:ALA:HA	2.50	0.46
1:A:938:GLY:O	1:A:942:THR:N	2.48	0.46
1:A:953:THR:H	1:A:958:TYR:HA	1.79	0.46
1:A:198:SER:O	1:A:202:GLU:CB	2.64	0.46
1:A:1369:PRO:HA	1:A:1370:PRO:HD3	1.82	0.46
1:A:1684:ALA:HB1	1:A:1688:GLN:HG2	1.98	0.46
1:A:534:ALA:HB2	1:A:558:MET:HE2	1.97	0.46
1:A:401:LYS:HA	1:A:404:GLN:HG2	1.96	0.46
1:A:2198:LYS:O	1:A:2202:HIS:CB	2.64	0.46
1:A:1040:LYS:O	1:A:1044:ALA:HB2	2.14	0.46
1:A:1817:ARG:O	1:A:1821:ASP:CB	2.58	0.45
1:A:276:ARG:O	1:A:279:SER:OG	2.31	0.45
1:A:588:TYR:HD1	1:A:593:PHE:HB3	1.81	0.45
1:A:299:GLN:HA	1:A:302:GLN:HB3	1.97	0.45
1:A:1610:ASN:HA	1:A:1613:ILE:HD12	1.99	0.45
1:A:2025:GLY:O	1:A:2029:ILE:CB	2.65	0.45
1:A:569:ILE:HG21	1:A:1383:MET:HE2	1.99	0.45
1:A:411:ASP:O	1:A:414:GLY:N	2.50	0.45
1:A:685:TRP:O	1:A:689:SER:CB	2.64	0.45
1:A:941:THR:O	1:A:945:ILE:CB	2.65	0.45
1:A:554:TYR:OH	1:A:597:GLN:NE2	2.50	0.45
1:A:578:PRO:HD3	1:A:627:TYR:CE1	2.52	0.45
1:A:744:ASN:HA	1:A:747:ALA:HB3	1.98	0.45
1:A:1358:VAL:HG11	1:A:1717:VAL:HG13	1.99	0.45
1:A:1379:LEU:HG	1:A:1632:PHE:CE1	2.53	0.44
1:A:2005:GLU:O	1:A:2009:PHE:CB	2.65	0.44
1:A:1448:LEU:HA	1:A:1451:ASN:HB2	2.00	0.44
1:A:1380:GLN:HE21	1:A:1603:SER:HB2	1.82	0.44
1:A:1040:LYS:O	1:A:1044:ALA:CB	2.66	0.44
1:A:1554:ALA:O	1:A:1558:MET:CB	2.66	0.44
1:A:63:SER:HB2	1:A:602:GLN:HG3	1.99	0.44
1:A:43:ARG:HE	1:A:632:PHE:HD2	1.65	0.43
1:A:365:SER:O	1:A:368:SER:OG	2.30	0.43
1:A:2080:ARG:O	1:A:2084:TRP:CB	2.66	0.43
1:A:219:ARG:O	1:A:223:ALA:CB	2.66	0.43
1:A:483:THR:OG1	1:A:484:TRP:N	2.51	0.43
1:A:445:ASN:O	1:A:449:TRP:CB	2.67	0.43
1:A:57:PRO:HG3	1:A:82:PHE:HE2	1.83	0.43
1:A:579:ARG:O	1:A:1596:ASN:ND2	2.52	0.43
1:A:388:ASP:OD1	1:A:388:ASP:N	2.45	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:ILE:O	1:A:757:LEU:HB2	2.19	0.43
1:A:1456:MET:HG2	1:A:1458:ASN:H	1.83	0.43
1:A:1770:LEU:HA	1:A:1773:VAL:HG12	2.01	0.43
1:A:1741:LEU:O	1:A:1745:TYR:CB	2.65	0.42
1:A:449:TRP:O	1:A:453:LEU:CB	2.68	0.42
1:A:1721:PHE:HA	1:A:1724:PHE:HB2	2.01	0.42
1:A:667:LEU:O	1:A:671:MET:HB2	2.19	0.42
1:A:1072:TRP:O	1:A:1076:LEU:CB	2.68	0.42
1:A:1623:ASN:HD21	1:A:1626:HIS:HD2	1.67	0.42
1:A:1749:ILE:HD13	1:A:1749:ILE:HG21	1.82	0.42
1:A:1775:LEU:HD23	1:A:1775:LEU:HA	1.90	0.42
1:A:1857:ALA:O	1:A:1860:GLY:N	2.52	0.42
1:A:596:LEU:HD13	1:A:596:LEU:HA	1.87	0.42
1:A:1590:VAL:HG21	1:A:1609:ILE:HD13	2.02	0.42
1:A:1535:PHE:HB3	1:A:1592:VAL:HA	2.01	0.42
1:A:1745:TYR:CZ	1:A:1749:ILE:HD11	2.54	0.42
1:A:223:ALA:O	1:A:227:ARG:N	2.53	0.42
1:A:1336:ARG:HG2	1:A:1705:TRP:CG	2.55	0.42
1:A:1866:ILE:O	1:A:1870:ILE:CB	2.68	0.42
1:A:386:THR:HG23	1:A:519:LEU:HD13	2.01	0.42
1:A:110:ARG:HG2	1:A:1545:LEU:HD12	2.02	0.41
1:A:560:ILE:HA	1:A:560:ILE:HD13	1.84	0.41
1:A:596:LEU:O	1:A:600:VAL:HB	2.20	0.41
1:A:1706:ASP:OD2	1:A:1754:TYR:OH	2.28	0.41
1:A:1358:VAL:HG22	1:A:1661:VAL:HG22	2.03	0.41
1:A:1555:ILE:O	1:A:1559:LYS:HB2	2.19	0.41
1:A:657:LYS:O	1:A:661:TYR:CB	2.68	0.41
1:A:667:LEU:HA	1:A:670:THR:HG22	2.03	0.41
1:A:1336:ARG:HG2	1:A:1705:TRP:CD1	2.56	0.41
1:A:1524:LYS:HZ1	1:A:1526:TRP:CD1	2.37	0.41
1:A:26:LEU:O	1:A:30:ALA:CB	2.69	0.41
1:A:82:PHE:HE1	1:A:312:PRO:HB2	1.86	0.41
1:A:672:ARG:NH1	1:A:678:ASN:OD1	2.48	0.41
1:A:1554:ALA:O	1:A:1558:MET:HB3	2.21	0.41
1:A:1686:HIS:O	1:A:1690:ILE:HG12	2.20	0.41
1:A:1954:SER:O	1:A:1958:MET:CB	2.69	0.41
1:A:1100:ARG:HA	1:A:1114:SER:HA	2.04	0.40
1:A:1385:ASN:OD1	1:A:1385:ASN:N	2.52	0.40
1:A:1638:LEU:HD23	1:A:1642:GLN:HB3	2.03	0.40
1:A:709:LEU:HA	1:A:709:LEU:HD12	1.83	0.40
1:A:1959:LEU:HA	1:A:1964:THR:HA	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ASN:HA	1:A:359:MET:HG2	2.02	0.40
1:A:552:VAL:HG21	1:A:604:ILE:HG21	2.02	0.40
1:A:1740:LEU:O	1:A:1744:LEU:CB	2.70	0.40
1:A:492:ASN:O	1:A:496:ARG:HG2	2.21	0.40
1:A:1697:ILE:O	1:A:1701:SER:OG	2.26	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	1869/2305 (81%)	1603 (86%)	263 (14%)	3 (0%)	43 76

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	2017	PRO
1	A	1461	PRO
1	A	1459	PRO

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	943/2027 (46%)	931 (99%)	12 (1%)	61 72

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	27	LEU
1	A	367	LEU
1	A	383	ILE
1	A	384	LEU
1	A	392	THR
1	A	533	TRP
1	A	548	LEU
1	A	596	LEU
1	A	767	TRP
1	A	1590	VAL
1	A	1636	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	ASN
1	A	51	GLN
1	A	96	ASN
1	A	134	GLN
1	A	361	ASN
1	A	1380	GLN
1	A	1450	GLN
1	A	1457	GLN
1	A	1458	ASN
1	A	1523	ASN
1	A	1552	ASN
1	A	1557	GLN
1	A	1610	ASN
1	A	1623	ASN
1	A	1641	GLN
1	A	1686	HIS
1	A	1726	GLN
1	A	1812	HIS

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 ⓘ

7 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	0.79	1 (7%)	17,19,21	0.66	0
2	NAG	B	2	2	14,14,15	0.71	1 (7%)	17,19,21	1.21	2 (11%)
2	BMA	B	3	2	11,11,12	0.60	0	15,15,17	0.82	1 (6%)
2	BMA	B	4	2	11,11,12	0.69	0	15,15,17	0.84	0
2	BMA	B	5	2	11,11,12	0.89	0	15,15,17	0.89	0
3	NAG	C	1	1,3	14,14,15	0.36	0	17,19,21	0.79	0
3	NAG	C	2	3	14,14,15	0.64	0	17,19,21	1.26	2 (11%)

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	-	1/6/23/26	0/1/1/1
2	NAG	B	2	2	-	4/6/23/26	0/1/1/1
2	BMA	B	3	2	-	2/2/19/22	0/1/1/1
2	BMA	B	4	2	-	0/2/19/22	0/1/1/1
2	BMA	B	5	2	-	2/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	C	2	3	-	4/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	NAG	O5-C1	-2.81	1.39	1.43
2	B	2	NAG	O5-C1	-2.32	1.39	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	2	NAG	C2-N2-C7	3.44	127.51	122.90
2	B	2	NAG	C2-N2-C7	3.17	127.14	122.90
2	B	2	NAG	C1-O5-C5	2.95	116.13	112.19
3	C	2	NAG	C1-C2-N2	2.18	113.88	110.43
2	B	3	BMA	O2-C2-C3	-2.06	105.89	110.15

There are no chirality outliers.

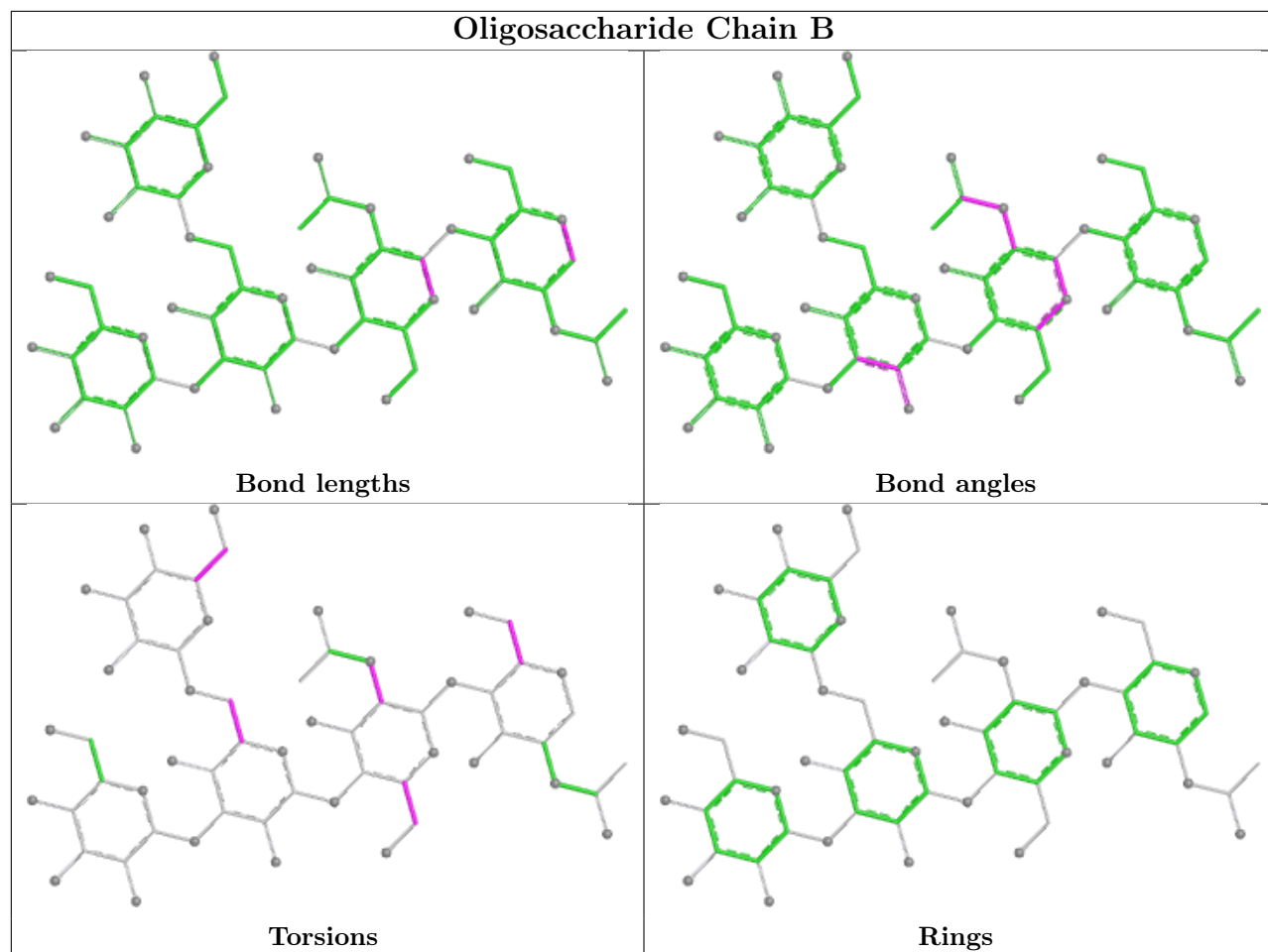
All (15) torsion outliers are listed below:

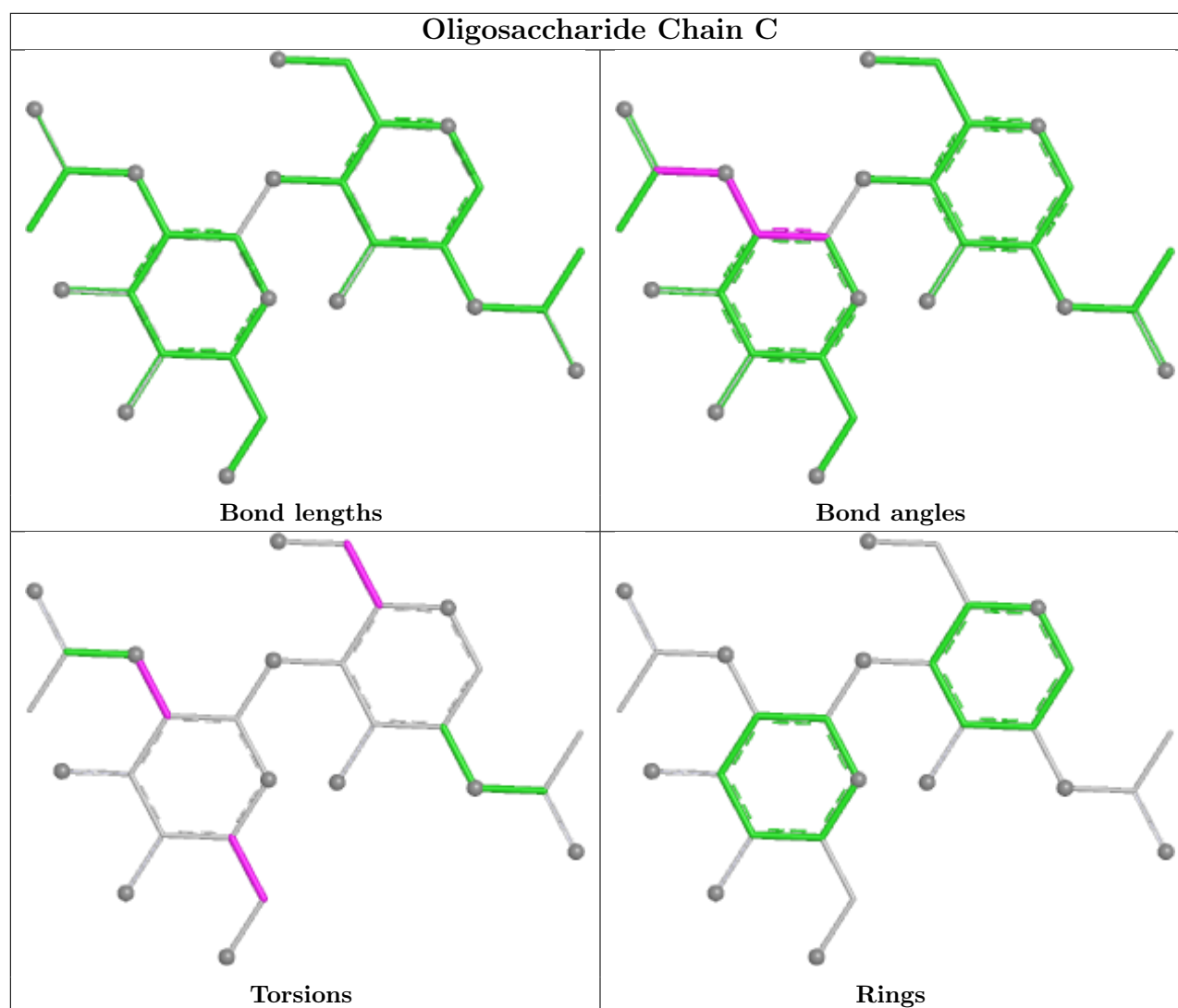
Mol	Chain	Res	Type	Atoms
2	B	5	BMA	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6
2	B	3	BMA	C4-C5-C6-O6
2	B	5	BMA	C4-C5-C6-O6
3	C	1	NAG	O5-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	C	1	NAG	C4-C5-C6-O6
2	B	2	NAG	O5-C5-C6-O6
2	B	3	BMA	O5-C5-C6-O6
2	B	1	NAG	O5-C5-C6-O6
3	C	2	NAG	C1-C2-N2-C7
2	B	2	NAG	C4-C5-C6-O6
3	C	2	NAG	C3-C2-N2-C7
2	B	2	NAG	C1-C2-N2-C7
2	B	2	NAG	C3-C2-N2-C7

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](#)

5 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	2305	1	14,14,15	0.83	2 (14%)	17,19,21	0.87	1 (5%)
4	NAG	A	2304	1	14,14,15	0.32	0	17,19,21	0.47	0
4	NAG	A	2303	1	14,14,15	0.25	0	17,19,21	0.38	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	A	2301	1	14,14,15	0.48	0	17,19,21	0.76	1 (5%)
4	NAG	A	2302	1	14,14,15	0.25	0	17,19,21	0.51	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	2305	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2304	1	-	1/6/23/26	0/1/1/1
4	NAG	A	2303	1	-	1/6/23/26	0/1/1/1
4	NAG	A	2301	1	-	2/6/23/26	0/1/1/1
4	NAG	A	2302	1	-	1/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2305	NAG	C1-C2	2.22	1.55	1.52
4	A	2305	NAG	O5-C1	2.11	1.47	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	2305	NAG	C1-O5-C5	2.82	115.97	112.19
4	A	2301	NAG	C1-O5-C5	2.70	115.81	112.19

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	2301	NAG	O5-C5-C6-O6
4	A	2301	NAG	C4-C5-C6-O6
4	A	2305	NAG	C8-C7-N2-C2
4	A	2305	NAG	O7-C7-N2-C2
4	A	2303	NAG	O5-C5-C6-O6
4	A	2304	NAG	O5-C5-C6-O6
4	A	2302	NAG	C1-C2-N2-C7

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.

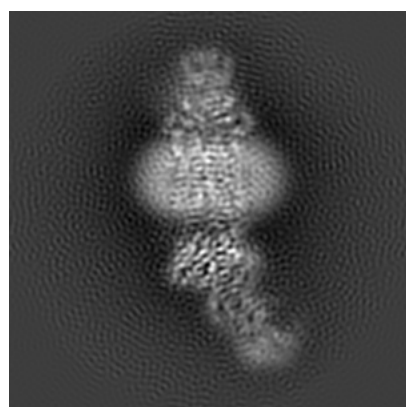
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6724. These allow visual inspection of the internal detail of the map and identification of artifacts.

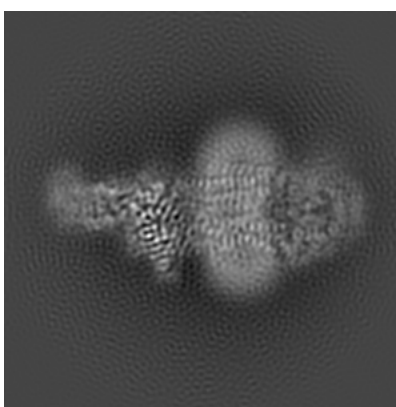
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

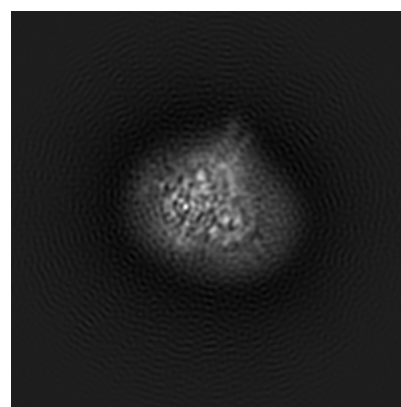
6.1.1 Primary map



X



Y

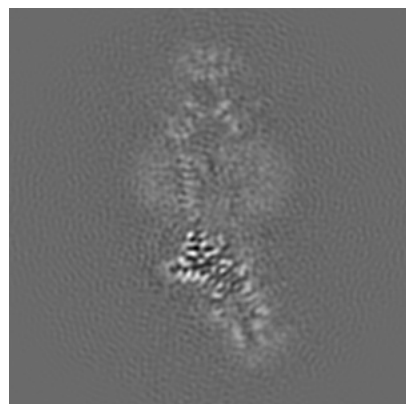


Z

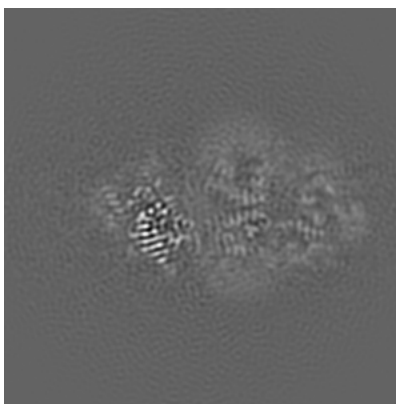
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

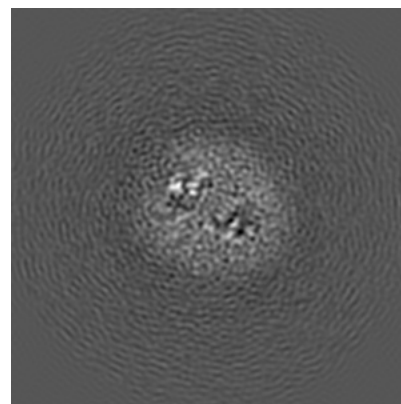
6.2.1 Primary map



X Index: 100



Y Index: 100

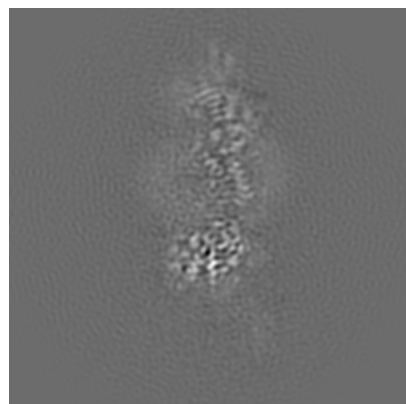


Z Index: 100

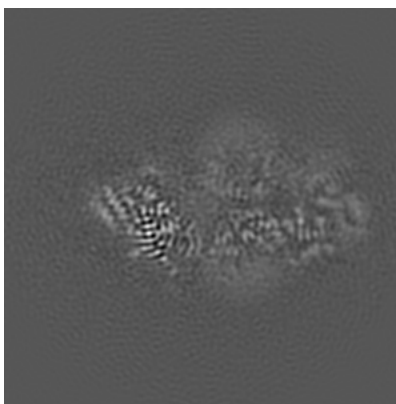
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

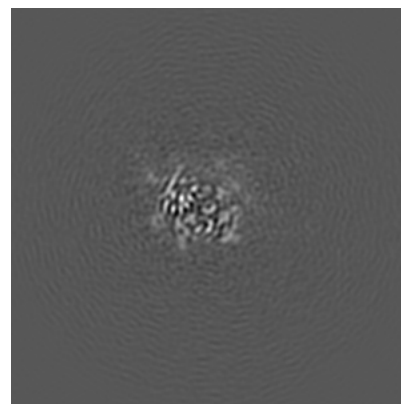
6.3.1 Primary map



X Index: 87



Y Index: 102

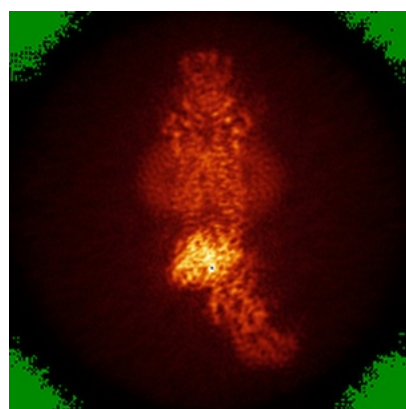


Z Index: 76

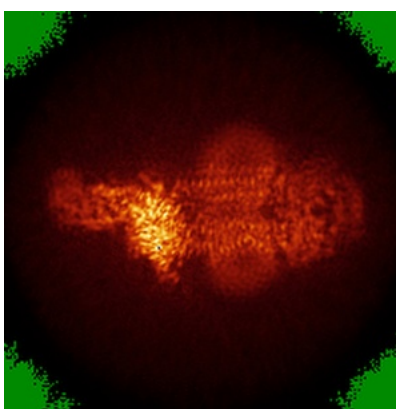
The images above show the largest variance slices of the map in three orthogonal directions.

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

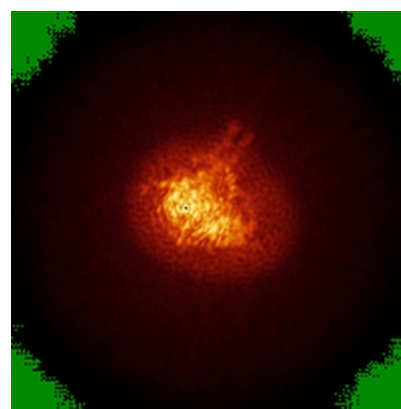
6.4.1 Primary map



X



Y



Z

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 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

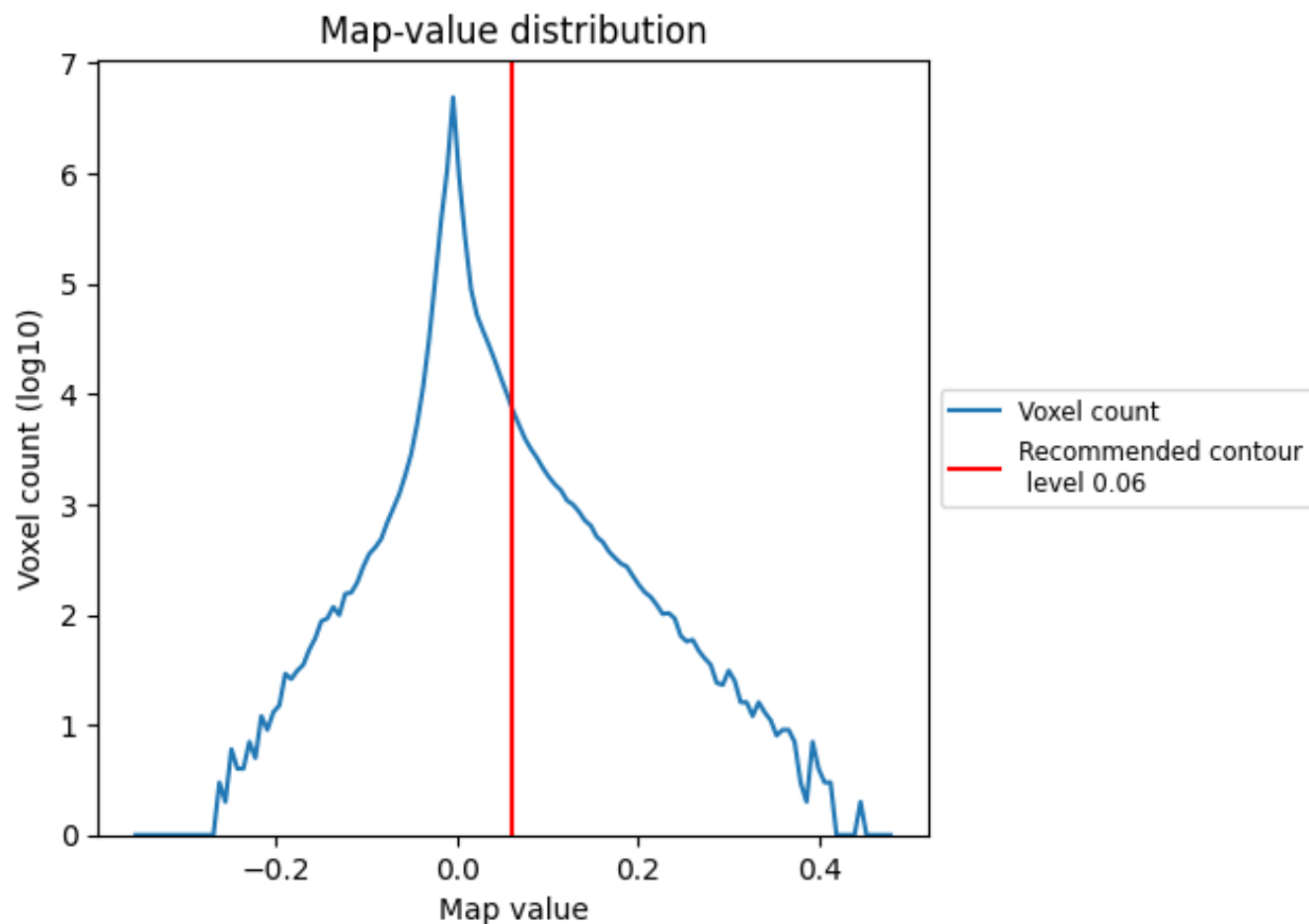
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

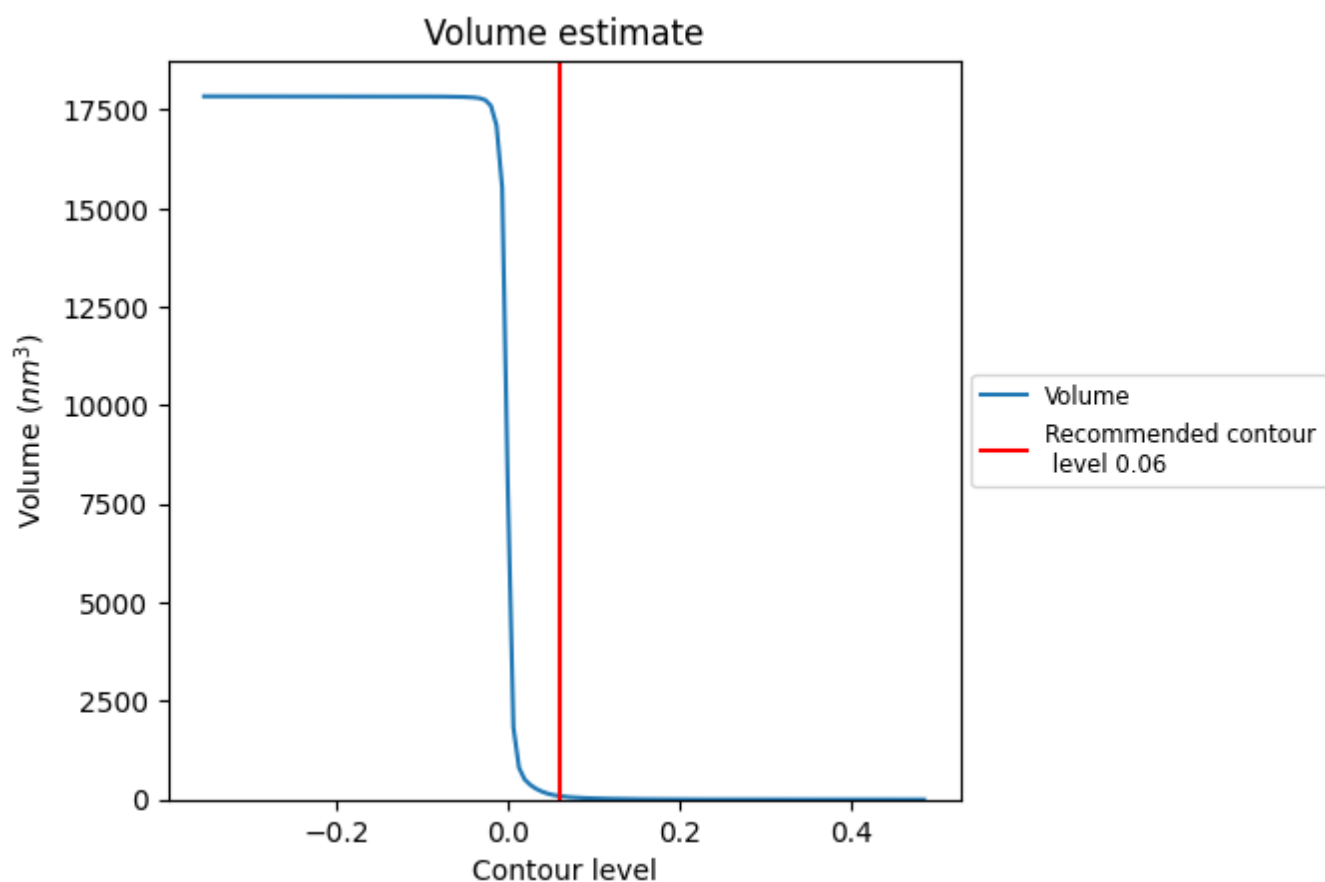
This section contains the results of statistical analysis of the map.

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.

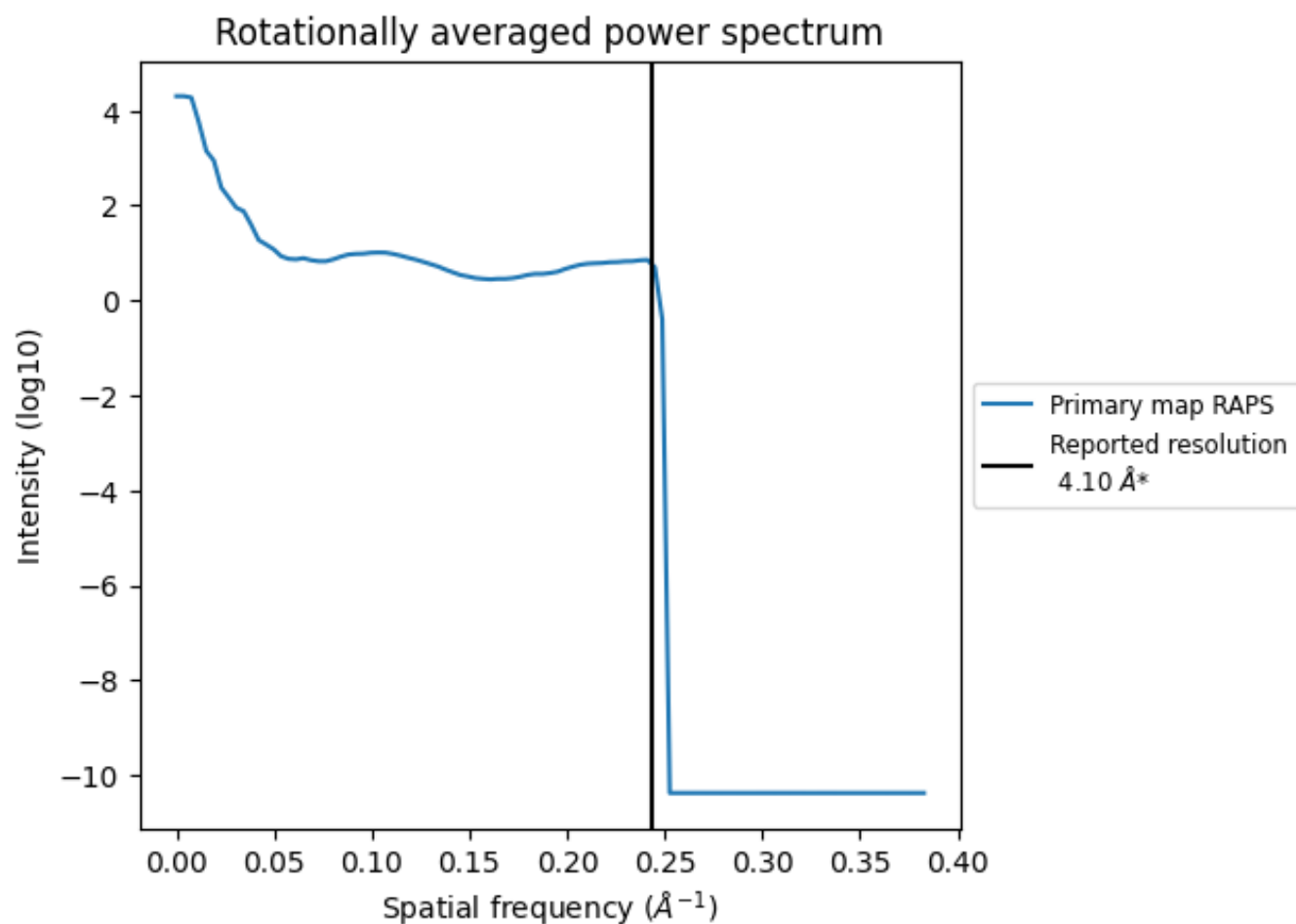
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 89 nm³; this corresponds to an approximate mass of 81 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 0.244 Å⁻¹

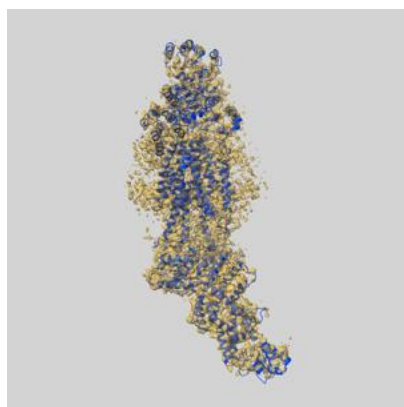
8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

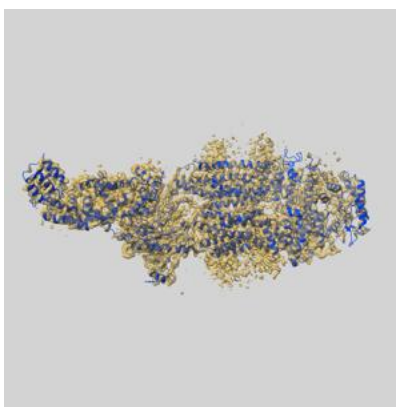
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-6724 and PDB model 5XJY. Per-residue inclusion information can be found in section [3](#) on page [6](#).

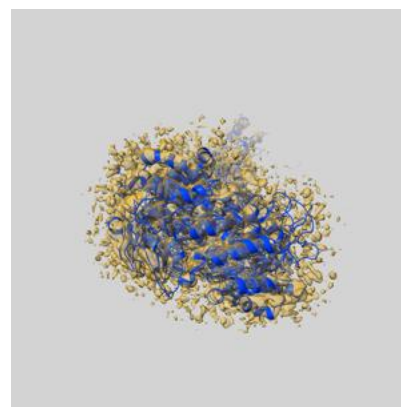
9.1 Map-model overlay [i](#)



X



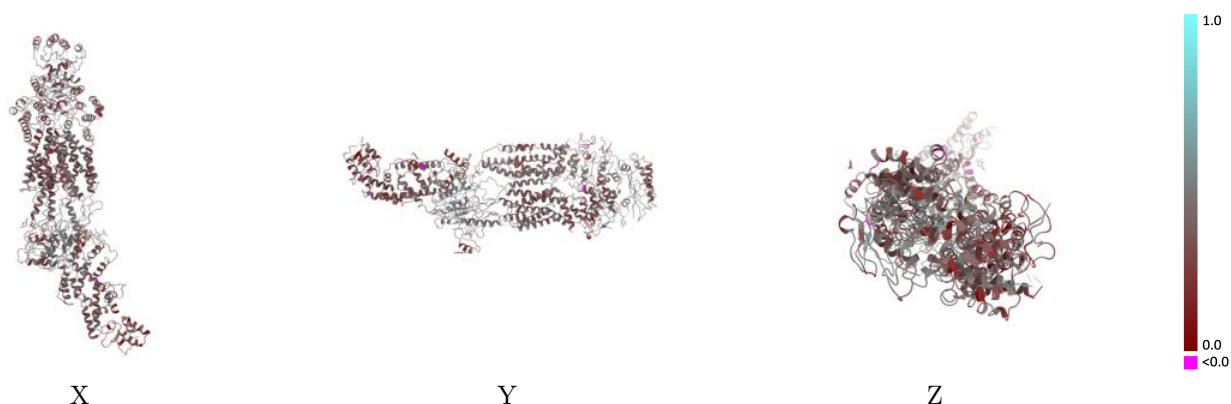
Y



Z

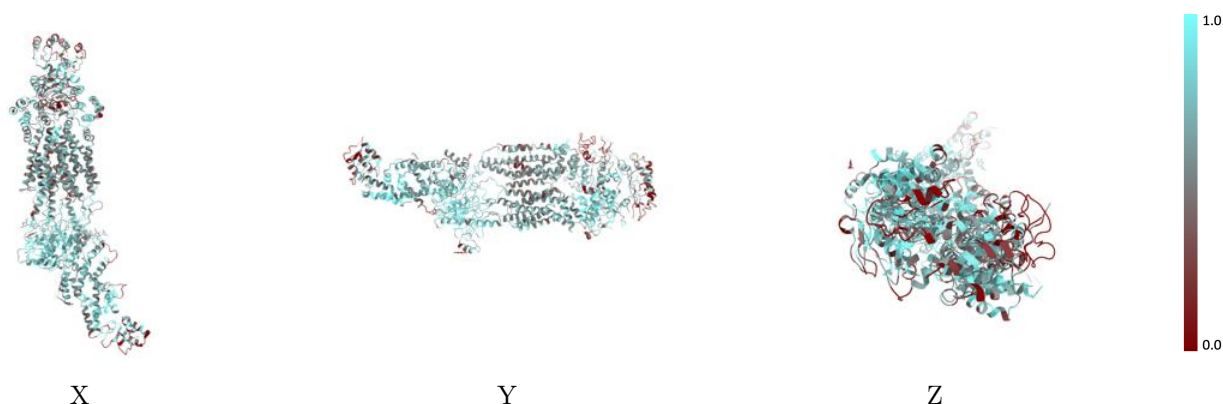
The images above show the 3D surface view of the map at the recommended contour level 0.06 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



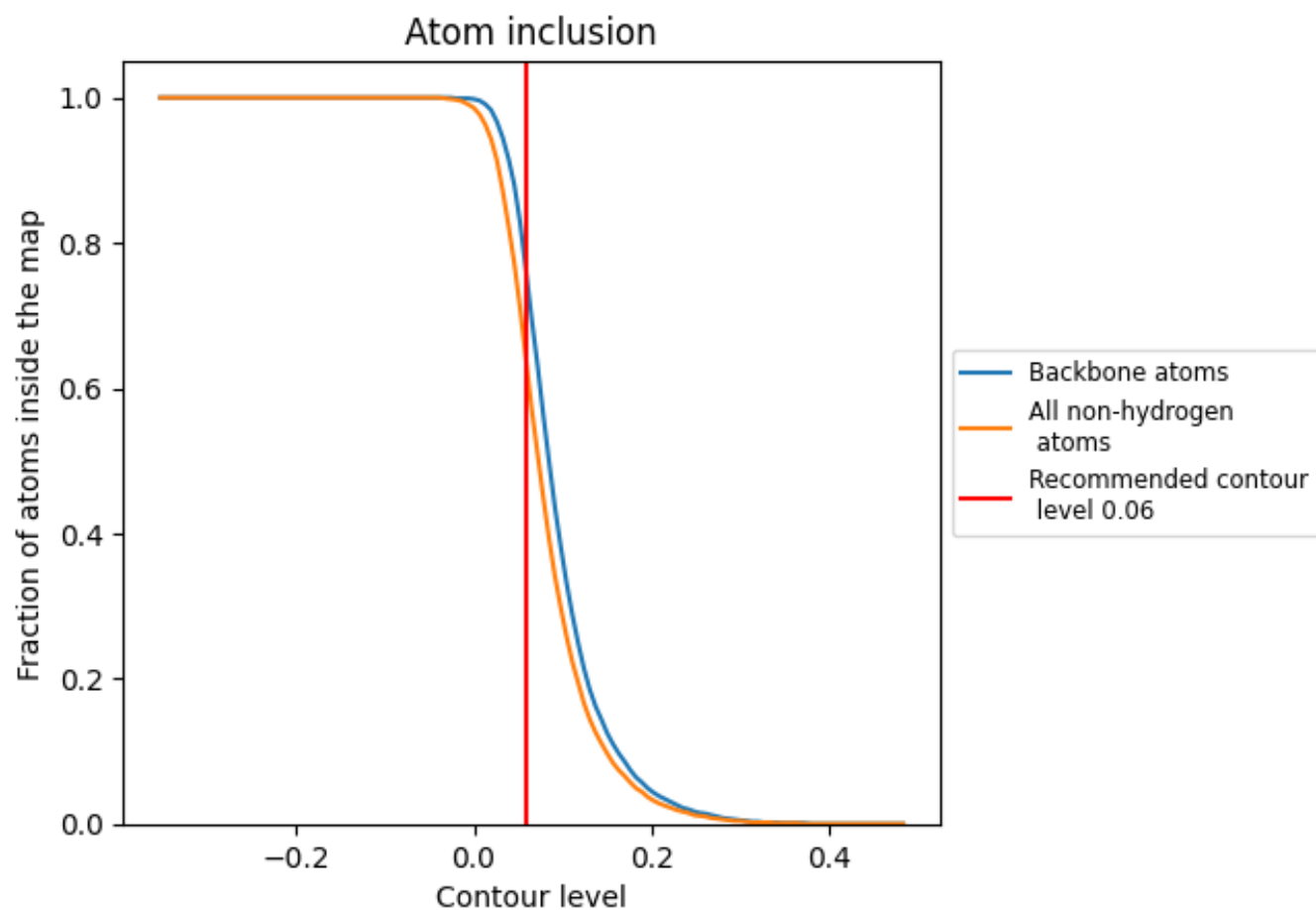
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.06).

9.4 Atom inclusion [i](#)



At the recommended contour level, 75% of all backbone atoms, 63% 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 (0.06) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6280	0.3870
A	0.6270	0.3860
B	0.7700	0.5080
C	0.6790	0.4410

