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PDB ID	:	5XJY
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 (i) 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 (i)) were used in the production of this report:

EMDB validation analysis	:	0.0.1. dev 43
Mogul	:	1.8.5 (274361), CSD as 541 be (2020)
MolProbity	:	4.02b-467
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 (i)

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	$egin{array}{c} { m Whole \ archive} \ (\#{ m Entries}) \end{array}$	${f EM} {f structures} \ (\#{f Entries})$
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 <=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 cl	nain
			19%	
1	A	2305	67%	15% • 18%
	D	_		
2	В	5	40%	60%
3	C	2	50%	50%



2 Entry composition (i)

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	А	1901	Total 12626	C 8005	N 2236	0 2328	S 57	0	0

There are 44 discrepancies between the modelled and reference sequences:

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



Chain	Residue	Modelled	Actual	Comment	Reference
А	2269	ASP	-	expression tag	UNP 095477
А	2270	ALA	-	expression tag	UNP 095477
А	2271	VAL	-	expression tag	UNP 095477
A	2272	GLU	-	expression tag	UNP 095477
А	2273	GLY	-	expression tag	UNP 095477
А	2274	SER	-	expression tag	UNP 095477
A	2275	HIS	-	expression tag	UNP 095477
А	2276	HIS	-	expression tag	UNP 095477
A	2277	HIS	-	expression tag	UNP 095477
А	2278	HIS	-	expression tag	UNP 095477
А	2279	HIS	-	expression tag	UNP 095477
А	2280	HIS	-	expression tag	UNP 095477
A	2281	HIS	-	expression tag	UNP 095477
A	2282	HIS	-	expression tag	UNP 095477
A	2283	HIS	-	expression tag	UNP 095477
A	2284	HIS	-	expression tag	UNP 095477

• Molecule 2 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[beta-D-mannopyranos e-(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	I	Aton	ns		AltConf	Trace
2	В	5	Total 61	С 34	N 2	O 25	0	0

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



Mol	Chain	Residues	I	Aton	ns		AltConf	Trace
3	С	2	Total 28	C 16	N 2	O 10	0	0

• Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).





Mol	Chain	Residues	Atoms	AltConf	
4	Λ	1	Total C N O	0	
4	Л	1	70 40 5 25	0	
4	Λ	1	Total C N O	0	
4		1	70 40 5 25	0	
4	Λ	1	Total C N O	0	
-1	Π	1	70 40 5 25	0	
4	Δ	1	Total C N O	0	
-1	Π	T	70 40 5 25	0	
4	Δ	1	Total C N O	0	
4	А	A	1	70 40 5 25	U



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: ATP-binding cassette sub-family A member 1







L2034	A2079 R2080 R2081 W2084 R2092 R2095 R2005	A21115 12116 M2117 V2118 V2119 G2120 R2121 F2122 R2123 R2123 R2123 R2123 R2123 R2135 R2135 R2135	TYR THR IIHR 2144 82144 ASP ISO ISO ISO ISO VAL
GLN ASP PHE F2159 2164 V2167 V2167 L2168 K2169 K2171	N2174 M2176 2179 22185 22185 22185 22185 22185 52185 52185 52195 52195 72191 72191 72193 12194 52195 72191	42196 42196 \$319 \$2196 \$12201 12201 \$12202 12202 \$12204 \$2204 \$2206 \$2208 \$2208 \$2208 \$2209 \$2208 \$2209 \$2208 \$2209 \$2208 \$2209 \$2208 \$2209 \$2209	T2211 T2212 L2213 D2214 Q2215 F2216 F2216 F2216 F2218 A1A A1A LVS A1A A1A A1A
GLN SER ASP ASP ASP ASP H2229 L222 LEU LEU LEU LYS CLN THR	VAL VAL ASP VAL ALA ALA ALA THR THR THR BER GLU GLU GLU GLU GLU GLU	SER SER ASP ALU VAL ALA ALA ALA ALA CLU CLU CLU CLU CLU CLU HIS HIS HIS HIS	HI S HI S HI S
• Molecule 2: beta-I -(1-4)-2-acetamido-2 se	D-mannopyranose-(1-3)-[beta-D 2-deoxy-beta-D-glucopyranose-(-mannopyranose-(1-6)]b 1-4)-2-acetamido-2-deox	eta-D-mannopyranose xy-beta-D-glucopyrano
Chain B:	40%	60%	

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

Chain C:	50%	50%
NAG1 NAG2		



4 Experimental information (i)

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	Depositor
	CORRECTION	
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 (i)

5.1 Standard geometry (i)

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).

Mal Chain		Bond lengths		Bond angles	
IVIOI	Unain	RMSZ	# Z > 5	RMSZ	# Z > 5
1	А	0.49	0/12840	0.69	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	А	0	15

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
1	А	1636	LEU	CA-CB-CG	8.43	134.69	115.30
1	А	367	LEU	CA-CB-CG	6.60	130.48	115.30
1	А	1497	LEU	CA-CB-CG	5.95	128.99	115.30
1	А	569	ILE	CG1-CB-CG2	-5.88	98.46	111.40
1	А	1815	LEU	CA-CB-CG	5.63	128.25	115.30
1	А	1398	ASP	CB-CG-OD1	5.40	123.16	118.30
1	А	1499	ASP	CB-CG-OD1	5.33	123.09	118.30
1	А	61	MET	CG-SD-CE	-5.18	91.91	100.20
1	А	378	LEU	CA-CB-CG	5.16	127.16	115.30

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	А	1427	THR	Peptide
Continued on next nage				



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

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	А	12626	0	10430	213	0
2	В	61	0	52	0	0
3	С	28	0	25	0	0
4	А	70	0	65	0	0
All	All	12785	0	10572	213	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 (213) 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



	Jus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	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:712:TYR:HH	1:A:1472:LYS:H	1.43	0.66
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: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: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:1524:LYS:HZ1	1:A:1526:TRP:HD1	1.53	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
1:A:9:LEU:HD21	1:A:996:PHE:HA	1.87	0.55



		Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
1:A:447:HIS:O	1:A:451:GLN:CB	2.53	0.55
1:A:1451:ASN:O	1:A:1455:THR:OG1	2.20	0.55
1:A:1456:MET:O	1:A:1460:SER:OG	2.23	0.55
1:A:88:GLY:O	1:A:1591:LYS:NZ	2.37	0.54
1:A:2017:PRO:O	1:A:2021:VAL:N	2.37	0.54
1:A:1684:ALA:HA	1:A:1687:LEU:HB3	1.88	0.54
1:A:12:TRP:O	1:A:16:THR:OG1	2.21	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:282:ARG:HA	1:A:285:VAL:HG22	1.91	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: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
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



		Interatomic	Clash
Atom-1	Atom-2	distance $(Å)$	overlap (Å)
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:641:PRO:O	1:A:645:THR:OG1	2.23	0.48
1:A:775:LEU:O	1:A:779:ALA:CB	2.61	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:1507:ASP:OD1	1:A:1511:LYS:NZ	2.41	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
1:A:1490:LYS:NZ	1:A:1492:ASN:OD1	2.39	0.47
1:A:199:LYS:O	1:A:203:MET:CB	2.62	0.46



	bus puge	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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: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:1727:LYS:NZ	1:A:1821:ASP:OD2	2.35	0.45
1:A:2025:GLY:O	1:A:2029:ILE:CB	2.65	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
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



	is page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
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: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
1:A:356:ASN:HA	1:A:359:MET:HG2	2.02	0.40
1:A:61:MET:HB3	1:A:61:MET:HE2	1.92	0.40
1:A:552:VAL:HG21	1:A:604:ILE:HG21	2.02	0.40



Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	А	1869/2305~(81%)	1603 (86%)	263 (14%)	3 (0%)	47 80

All (3) Ramachandran outliers are listed below:

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

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent side chain 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	А	943/2027~(46%)	929~(98%)	14 (2%)	65 79	

All (14) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	А	27	LEU
1	А	96	ASN
1	А	373	LYS
1	А	383	ILE
1	А	384	LEU
1	А	533	TRP
1	А	638	ARG
1	А	767	TRP
1	А	1417	ARG
1	А	1456	MET
1	А	1458	ASN
1	А	1472	LYS
1	А	1523	ASN
1	А	1552	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	А	14	ASN
1	А	96	ASN
1	А	597	GLN
1	А	621	GLN
1	А	1380	GLN
1	А	1450	GLN
1	А	1458	ASN
1	А	1523	ASN
1	А	1552	ASN
1	А	1557	GLN
1	А	1607	ASN
1	А	1610	ASN
1	А	1623	ASN
1	А	1734	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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



5.5 Carbohydrates (i)

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).

Mal	Turne	Chain	Dec	Tink	Bo	ond leng	\mathbf{ths}	B	ond ang	les
IVIOI	туре	Unam	nes	LIIIK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
2	NAG	В	1	2,1	$14,\!14,\!15$	0.83	1 (7%)	17,19,21	0.65	0
2	NAG	В	2	2	14,14,15	0.73	1 (7%)	17,19,21	1.16	2 (11%)
2	BMA	В	3	2	11,11,12	0.62	0	15,15,17	0.88	1 (6%)
2	BMA	В	4	2	11,11,12	0.71	0	15,15,17	0.90	0
2	BMA	В	5	2	11,11,12	0.91	0	15,15,17	0.95	0
3	NAG	С	1	3,1	14,14,15	0.36	0	17,19,21	0.77	0
3	NAG	С	2	3	14,14,15	0.65	0	17,19,21	1.20	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	В	1	2,1	-	1/6/23/26	0/1/1/1
2	NAG	В	2	2	-	3/6/23/26	0/1/1/1
2	BMA	В	3	2	-	2/2/19/22	0/1/1/1
2	BMA	В	4	2	-	0/2/19/22	0/1/1/1
2	BMA	В	5	2	-	2/2/19/22	0/1/1/1
3	NAG	С	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	С	2	3	-	3/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	$\mathrm{Ideal}(\mathrm{\AA})$
2	В	1	NAG	O5-C1	-2.97	1.39	1.43
2	В	2	NAG	O5-C1	-2.45	1.39	1.43

All (4) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Ζ	$\mathbf{Observed}(^{o})$	$Ideal(^{o})$
3	С	2	NAG	C2-N2-C7	3.23	127.51	122.90
2	В	2	NAG	C2-N2-C7	2.98	127.14	122.90
2	В	2	NAG	C1-O5-C5	2.91	116.13	112.19
2	В	3	BMA	O2-C2-C3	-2.12	105.89	110.14

There are no chirality outliers.

Mol	Chain	\mathbf{Res}	Type	Atoms
2	В	5	BMA	O5-C5-C6-O6
3	С	2	NAG	C4-C5-C6-O6
2	В	3	BMA	C4-C5-C6-O6
2	В	5	BMA	C4-C5-C6-O6
3	С	2	NAG	O5-C5-C6-O6
3	С	1	NAG	O5-C5-C6-O6
3	С	1	NAG	C4-C5-C6-O6
2	В	2	NAG	O5-C5-C6-O6
2	В	3	BMA	O5-C5-C6-O6
2	В	1	NAG	O5-C5-C6-O6
2	В	2	NAG	C4-C5-C6-O6
3	С	2	NAG	C3-C2-N2-C7
2	В	2	NAG	C3-C2-N2-C7

All (13) torsion outliers are listed below:

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).

Mal	Turne	Chain	Dec	Tink	Bo	ond leng	$_{\rm ths}$	В	ond ang	les
WIOI	туре	Unam	nes		Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	А	2305	1	14,14,15	0.82	2 (14%)	17,19,21	0.85	1 (5%)
4	NAG	А	2301	1	14,14,15	0.48	0	17,19,21	0.74	1 (5%)
4	NAG	А	2303	1	14,14,15	0.25	0	17,19,21	0.37	0



Mal	Turne	Chain	Dec	Tink	Bo	ond leng	\mathbf{ths}	В	ond ang	les
IVIOI	туре	Unam	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z >2
4	NAG	А	2302	1	14,14,15	0.24	0	17,19,21	0.49	0
4	NAG	А	2304	1	14,14,15	0.30	0	17,19,21	0.45	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	А	2305	1	-	2/6/23/26	0/1/1/1
4	NAG	А	2301	1	-	2/6/23/26	0/1/1/1
4	NAG	А	2303	1	-	1/6/23/26	0/1/1/1
4	NAG	А	2302	1	-	0/6/23/26	0/1/1/1
4	NAG	А	2304	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)	$\mathrm{Ideal}(\mathrm{\AA})$
4	А	2305	NAG	O5-C1	2.21	1.47	1.43
4	А	2305	NAG	C1-C2	2.03	1.55	1.52

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
4	А	2305	NAG	C1-O5-C5	2.79	115.97	112.19
4	А	2301	NAG	C1-O5-C5	2.67	115.81	112.19

There are no chirality outliers.

All (6) torsion outliers are listed below:

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

There are no ring outliers.

No monomer is involved in short contacts.



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-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.

Orthogonal projections (i) 6.1

6.1.1Primary map



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

Central slices (i) 6.2

6.2.1Primary map



X Index: 100

Y 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 surface views (i)

6.4.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.06. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.



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 89 nm^3 ; 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 (i)



*Reported resolution corresponds to spatial frequency of 0.244 $\rm \AA^{-1}$



8 Fourier-Shell correlation (i)

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)



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 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 (i)

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	0.6276	0.3870
А	0.6268	0.3860
В	0.7705	0.5080
С	0.6786	0.4410



