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PDB ID	:	8ZJF
EMDB ID	:	EMD-60143
Title	:	Cryo-EM structure of human integrin alpha-E beta-7
Authors	:	Akasaka, H.; Nureki, O.; Kise, Y.
Deposited on	:	2024-05-14
Resolution	:	2.70 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 92
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	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.70 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.



INTEGI IC	$(\# { m Entries})$	$(\# { m Entries})$
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 chain				
1	В	826	46%	16%		38%	
2	А	1198	57%		16%	•	24%
3	С	3	67%			33	3%



2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 10917 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 Integrin beta-7.

Mol	Chain	Residues	Atoms			AltConf	Trace		
1	В	510	Total 3882	C 2390	N 704	0 754	S 34	0	0

There are 29 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
В	799	GLY	-	expression tag	UNP P26010
В	800	SER	-	expression tag	UNP P26010
В	801	GLY	-	expression tag	UNP P26010
В	802	SER	-	expression tag	UNP P26010
В	803	GLY	-	expression tag	UNP P26010
В	804	LEU	-	expression tag	UNP P26010
В	805	ASN	-	expression tag	UNP P26010
В	806	ASP	-	expression tag	UNP P26010
В	807	ILE	-	expression tag	UNP P26010
В	808	PHE	-	expression tag	UNP P26010
В	809	GLU	-	expression tag	UNP P26010
В	810	ALA	-	expression tag	UNP P26010
В	811	GLN	-	expression tag	UNP P26010
В	812	LYS	-	expression tag	UNP P26010
В	813	ILE	-	expression tag	UNP P26010
В	814	GLU	-	expression tag	UNP P26010
В	815	TRP	-	expression tag	UNP P26010
В	816	HIS	-	expression tag	UNP P26010
В	817	GLU	-	expression tag	UNP P26010
В	818	GLY	-	expression tag	UNP P26010
В	819	SER	-	expression tag	UNP P26010
В	820	GLY	-	expression tag	UNP P26010
В	821	SER	-	expression tag	UNP P26010
В	822	GLU	-	expression tag	UNP P26010
В	823	ASN	-	expression tag	UNP P26010
В	824	LEU	-	expression tag	UNP P26010
В	825	TYR	-	expression tag	UNP P26010
В	826	PHE	-	expression tag	UNP P26010



Chain	Residue	ne Modelled Actual Comment		Reference	
В	827	GLN	-	expression tag	UNP P26010

• Molecule 2 is a protein called Integrin alpha-E.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Λ	000	Total	С	Ν	Ο	\mathbf{S}	0	0
	A	909	6993	4388	1225	1341	39	0	0

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
А	1180	LEU	-	expression tag	UNP P38570
А	1181	GLU	-	expression tag	UNP P38570
А	1182	LEU	-	expression tag	UNP P38570
А	1183	GLU	-	expression tag	UNP P38570
А	1184	VAL	-	expression tag	UNP P38570
А	1185	LEU	-	expression tag	UNP P38570
А	1186	PHE	-	expression tag	UNP P38570
А	1187	GLN	-	expression tag	UNP P38570
А	1188	GLY	-	expression tag	UNP P38570
А	1189	PRO	-	expression tag	UNP P38570
А	1190	GLY	-	expression tag	UNP P38570
А	1191	SER	-	expression tag	UNP P38570
А	1192	ASP	-	expression tag	UNP P38570
А	1193	TYR	-	expression tag	UNP P38570
А	1194	LYS	-	expression tag	UNP P38570
А	1195	ASP	-	expression tag	UNP P38570
А	1196	ASP	-	expression tag	UNP P38570
А	1197	ASP	-	expression tag	UNP P38570
А	1198	ASP	-	expression tag	UNP P38570
А	1199	LYS	-	expression tag	UNP P38570

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



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



• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	AltConf
4	В	1	Total Mg 1 1	0

• Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
5	В	2	Total Ca 2 2	0



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 = 2and 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: Integrin beta-7



GLU ASN LEU TYR PHE GLN

• Molecule 2: Integrin alpha-E

Chain A:

57%

24%



TRP	LEU	SIH	THR	TEU	CYS	ALA	SER	ALA	LEU LEU	ALA	ALA F10	NZO	u Cg	P26	W27	VEV	P35	.	S39	S40	L41 L42	153	L54	V55	P58	L67	H68 D60	CT0	D75		K89	V97	V98 R99		R113 R114	E121		41.30 1 1 1 2 0	0717
-	D151 A152	R153	V154	T156	G157 D158	CAS	TYR SER	ASN	GLU	GLY	GLY GLY	GLU	ASP	VAL	ASN TUP	ALA	ARG	GLN	ARG	ALA LEU	GLU	GLU	GLU	0TD	ASP	GLU	GLU GLU	GLU	GLU	GLU 5106	0	T201	1206	1013	D214	P215 P216	D217	R220 A221	
K222	N227	M228	N031		K235 C236	5237 F237	E238 C239		V244 0245	2 2 2	G248 V749	017 A	E253	L256	ogud	V269	Q270	1271 1272	T273	8277	V278	T279 K280		982W	L289	1292	S299	R300	A303	anana A	N306 M307	V308 V200	v 303 L310	1.306		K330 M331	E.335	R336 F337	
A338	1339 1	F345	R340	T350	A351 R352	E353	L354	1357	A358 S359		E363 T364	H365	A366	L378	Cocd	Y384	N385	1386 1387	S388	M389	0403	V421		F424 D425	W426	D452	R482	0011	H480	F490	K494	B407	E498	A499 S500	F501	Y513	S516	E517 E518 L518	
C519	M525		L533	D557	RE76		D586 L587	S588	D594		L601 FEDO	1001	D608	V616		N619	H621	W622	0624 G624		2020	G651	S656	G657 D658		D662	V673 E67A		V680 R681		A687	R704	L705	S711	T714	A715	E717	S718 G719	L720
R721	L725		L729	R739	U745		R753 E754	W755	S756	87 <mark>59</mark>	F763	204	P769	E773	E-1-1-1		S781	K786	V787	0620	L791	Q792	T798	008H	D803	I 804	L805	Y808	1814	F815	OTON	E820	K826	CR29		V839	<mark>0842</mark>	V845 V846	
G847	L848	L852	T853 1854	N855	I856 N857		D864 S865	Y866	M867 T868	S869	M870	L872	N873 V874	10/14 P875	R876	N877 1878	Q879	L880	R882	M883	ue884 K885	P886	P889	N890 T891	1892 0892	C893 D894	D895	P898	N899	L903	1904 M905	• 906N	C907	1909	G910 H911	P912	V913 L914	H920	-
V923	V924 W925	0926	L927 F038	E929		R935 T936	A937	T944	N945	S946	R950	S951	H957	T958	0960 0960	F961	R962 H963	G964	PHE VAL	ALA	VAL	SER	LYS PRO	SER	MET	TYR	ASN	GLY	GLN	LEU	SER	SIH	LYS	PHE	LEU PHE	HIS VAT	ALL	GLY GLY	ASN
LEU	PHE GLY	ALA	GLU TVR	GLN	LEU GI N	ILE	CYS VAL	PRO	THR	TEU	ARG GI V	TEU	GLN	VAL	AL.A	LYS	LYS	THR	ARG	GLN	ALA	SER THR	VAL	THR	TRP SFR	GLN	GLU ARG	ALA	ALA	TYR	SER	VAL	SIH	VAL	GTN	TRP HIS	SER VAL	SER	
VAL	ILE ALA	SER	ASP I VS	GLU	ASN VAL	THR	VAL ALA	ALA	GLU TLE	SER	TRP	HIS	SER	GLU	LEU	LYS	ASP	VAL THR	GLU	GLN	ILE	GLY	GLU	SER	PHE	TYS	SER LEU	TYR	GLY	LEU	ALA	GLU	SIH	ARG THR	TAS	THR	VAL. VAL.	PHE	
LYS	ASP GLU	LYS	TYR HTS	SER	LEU PRO	ILE	ILE	LYS	GLY SER	VAL	GLY GLY	TEU	LEU	LEU	ILE	ILE	LEU	VAL TLE	TEU	PHE	CYS	GLY	PHE	ARG	LYS TVR	GLN	GLN	ASN	GLU	SER	ARG	LYS	GLN	LEU	SER	GLU	LEU	GLU	
GLU	ASN LEU	GLU	LEU	VAL	LEU PHF	GLN	GLY PRO	GLY	ASP	TYR	LYS	ASP	ASP	LYS																									

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

67%

Chain C:

33%





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	300397	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE	Depositor
	CORRECTION	
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose $(e^-/\text{\AA}^2)$	50.855	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	1600	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.425	Depositor
Minimum map value	-0.958	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.027	Depositor
Recommended contour level	0.012	Depositor
Map size (Å)	233.1, 233.1, 233.1	wwPDB
Map dimensions	210, 210, 210	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.11, 1.11, 1.11	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: MG, CA, 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			
1VIOI	Chain	RMSZ	# Z > 5	RMSZ	# Z > 5		
1	В	0.25	0/3961	0.53	0/5368		
2	А	0.26	0/7136	0.53	1/9682~(0.0%)		
All	All	0.26	0/11097	0.53	1/15050~(0.0%)		

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	$Observed(^{o})$	$Ideal(^{o})$
2	А	867	MET	CA-CB-CG	5.60	122.83	113.30

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	В	3882	0	3740	76	0
2	А	6993	0	6853	129	0
3	С	39	0	34	1	0
4	В	1	0	0	0	0
5	В	2	0	0	0	0
All	All	10917	0	10627	201	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 (201) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom 1	Atom 2	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:A:721:ARG:HA	2:A:756:SER:HA	1.57	0.83
1:B:482:GLN:HB2	1:B:485:ALA:HB2	1.65	0.78
2:A:880:LEU:HD21	2:A:923:VAL:HG23	1.68	0.76
2:A:886:PRO:HB3	2:A:920:HIS:H	1.51	0.76
2:A:201:THR:HB	2:A:239:CYS:HB2	1.69	0.75
2:A:820:GLU:HB2	2:A:826:LYS:HG2	1.71	0.71
2:A:842:GLN:NE2	2:A:960:GLN:O	2.24	0.70
1:B:78:ARG:NH2	1:B:545:CYS:SG	2.65	0.69
1:B:137:PRO:HD3	1:B:444:GLN:HE22	1.57	0.69
2:A:364:THR:HG22	2:A:385:ASN:HD22	1.60	0.67
2:A:910:GLY:HA2	2:A:914:LEU:HD22	1.75	0.67
1:B:66:GLN:HB2	1:B:91:CYS:HB3	1.77	0.66
1:B:455:LEU:HB3	1:B:468:VAL:HB	1.76	0.66
2:A:227:ASN:O	2:A:231:ASN:ND2	2.29	0.65
2:A:790:GLN:OE1	2:A:792:GLN:NE2	2.29	0.65
1:B:297:ASP:OD1	2:A:513:TYR:OH	2.14	0.64
1:B:269:ALA:O	1:B:272:GLN:NE2	2.31	0.63
1:B:452:PRO:HB3	1:B:471:HIS:CE1	2.33	0.63
2:A:222:LYS:HD3	2:A:270:GLN:HA	1.81	0.63
2:A:38:LEU:HG	2:A:58:PRO:HD3	1.82	0.62
2:A:935:ARG:HH12	2:A:961:PHE:HE2	1.48	0.62
1:B:300:LEU:O	2:A:403:GLN:NE2	2.32	0.62
2:A:687:ALA:HB3	2:A:704:ARG:HB3	1.82	0.61
1:B:78:ARG:HH12	1:B:89:ARG:HH12	1.48	0.61
1:B:152:VAL:HG12	1:B:186:THR:HG21	1.83	0.61
1:B:523:LEU:HD12	1:B:524:GLU:HG2	1.83	0.61
2:A:786:LYS:HG3	2:A:814:ILE:HG13	1.82	0.61
1:B:203:PRO:HB2	2:A:426:TRP:HZ2	1.65	0.60
1:B:457:LEU:HD12	1:B:466:LEU:HD12	1.83	0.60
2:A:354:LEU:HA	2:A:357:ILE:HD12	1.83	0.60
1:B:83:ARG:NH1	1:B:98:GLU:OE2	2.35	0.60
1:B:47:PRO:HB3	1:B:78:ARG:HA	1.84	0.59
2:A:852:LEU:O	2:A:925:TRP:N	2.35	0.59
1:B:224:GLN:NE2	1:B:250:SER:O	2.36	0.59
1:B:106:LEU:HD12	1:B:127:ARG:HG2	1.85	0.59
1:B:190:ARG:NH2	1:B:276:GLY:O	2.35	0.59
2:A:739:ARG:NH2	2:A:781:SER:OG	2.36	0.58
1:B:341:ASN:OD1	1:B:458:ARG:NH1	2.36	0.58



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		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:B:262:PHE:HB3	1:B:328:PRO:HG2	1.85	0.58		
2:A:206:ILE:HD12	2:A:309:VAL:HG22	1.85	0.57		
2:A:235:LYS:HE3	2:A:383:ARG:HH21	1.70	0.57		
2:A:867:MET:HG2	2:A:946:SER:HB2	1.86	0.56		
1:B:65:LYS:HD2	1:B:480:ASP:HB2	1.88	0.56		
1:B:92:PRO:HD2	1:B:95:GLU:HB2	1.87	0.56		
2:A:494:LYS:HG3	2:A:499:ALA:HB2	1.88	0.55		
2:A:720:LEU:HD21	2:A:791:LEU:HD11	1.89	0.55		
2:A:34:ALA:HB3	2:A:35:PRO:HD3	1.88	0.55		
2:A:878:LEU:HD12	2:A:925:TRP:CG	2.41	0.54		
2:A:857:ASN:HB3	2:A:920:HIS:HD1	1.72	0.54		
2:A:898:PRO:HA	2:A:903:LEU:HD11	1.89	0.54		
1:B:127:ARG:NH1	1:B:469:GLU:OE2	2.36	0.54		
1:B:154:LEU:HD13	1:B:182:LEU:HD11	1.90	0.54		
2:A:869:SER:N	2:A:944:THR:O	2.37	0.54		
2:A:845:VAL:HG12	2:A:846:VAL:H	1.73	0.53		
1:B:58:HIS:O	1:B:133:ARG:NH2	2.42	0.53		
1:B:496:GLN:O	1:B:497:CYS:SG	2.63	0.53		
2:A:53:LEU:HB3	2:A:70:CYS:HB2	1.90	0.53		
2:A:245:GLN:NE2	2:A:273:THR:O	2.36	0.53		
2:A:20:ASN:ND2	2:A:588:SER:HA	2.23	0.53		
2:A:662:ASP:HB2	2:A:674:PHE:O	2.09	0.53		
2:A:718:SER:HB2	2:A:800:HIS:HB2	1.91	0.53		
2:A:895:ASP:N	2:A:895:ASP:OD1	2.42	0.53		
2:A:300:ARG:HB2	2:A:303:ALA:HB2	1.90	0.52		
2:A:594:ASP:HB3	2:A:619:ASN:HA	1.90	0.52		
2:A:865:SER:HB3	2:A:914:LEU:HD23	1.90	0.52		
1:B:410:SER:HB3	1:B:428:CYS:SG	2.50	0.52		
2:A:244:VAL:HG13	2:A:292:ILE:HD11	1.92	0.52		
2:A:889:PRO:HG2	2:A:891:ILE:HG13	1.92	0.52		
2:A:363:GLU:HG2	2:A:366:ALA:HB3	1.92	0.52		
1:B:215:PRO:HG3	1:B:226:PRO:HD3	1.91	0.51		
2:A:680:VAL:HG23	2:A:805:LEU:HD23	1.92	0.51		
2:A:681:ARG:H	2:A:711:SER:HB3	1.75	0.51		
1:B:131:THR:HG22	1:B:473:LEU:HB2	1.93	0.51		
2:A:278:VAL:HG13	2:A:280:LYS:HG3	1.93	0.51		
2:A:769:PRO:HB2	2:A:773:GLU:HB2	1.93	0.51		
2:A:359:SER:O	2:A:365:HIS:ND1	2.44	0.51		
2:A:899:VAL:HG12	2:A:903:LEU:HD13	1.92	0.51		
2:A:857:ASN:OD1	2:A:857:ASN:N	2.44	0.50		
2:A:519:CYS:HB3	2:A:533:LEU:HB2	1.92	0.50		



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	ious page	Interatomic	Clash	
Atom-1	Atom-2	distance (Å)	overlap (Å)	
1:B:85:GLU:O	1:B:89:ARG:NE	2.34	0.50	
2:A:854:LEU:HD22	2:A:925:TRP:HZ3	1.76	0.50	
2:A:602:GLU:OE2	2:A:616:TYR:OH	2.26	0.50	
2:A:854:LEU:HD23	2:A:856:ILE:HD11	1.93	0.50	
2:A:878:LEU:HA	2:A:927:LEU:HA	1.93	0.50	
1:B:412:CYS:HB3	1:B:437:VAL:HB	1.93	0.49	
1:B:374:ASP:N	1:B:374:ASP:OD1	2.45	0.49	
1:B:74:GLU:OE2	1:B:78:ARG:NH2	2.46	0.49	
2:A:27:TRP:HB2	2:A:673:VAL:HB	1.94	0.49	
2:A:42:LEU:HD12	2:A:651:GLY:HA2	1.94	0.49	
1:B:507:LEU:HB3	1:B:514:SER:HA	1.93	0.49	
1:B:287:THR:HG22	1:B:347:ALA:HB3	1.94	0.49	
1:B:547:ARG:HG3	1:B:557:HIS:HB2	1.93	0.49	
2:A:935:ARG:NH2	2:A:959:LEU:HB3	2.28	0.49	
2:A:236:CYS:SG	2:A:237:PHE:N	2.86	0.49	
2:A:25:ARG:NH2	2:A:75:ASP:OD2	2.46	0.48	
2:A:285:MET:O	2:A:289:LEU:HG	2.13	0.48	
1:B:489:SER:OG	1:B:501:SER:O	2.31	0.48	
2:A:331:MET:N	2:A:331:MET:HE2	2.28	0.48	
2:A:214:ASP:N	2:A:214:ASP:OD1	2.47	0.48	
2:A:872:LEU:HB3	2:A:905:MET:HB2	1.95	0.48	
2:A:557:ASP:N	2:A:557:ASP:OD1	2.47	0.47	
1:B:65:LYS:HD3	1:B:478:CYS:HB2	1.95	0.47	
1:B:380:GLN:NE2	1:B:384:ASP:OD1	2.47	0.47	
1:B:401:PRO:HD3	1:B:453:HIS:CE1	2.49	0.47	
1:B:156:TYR:HE1	1:B:158:MET:HG3	1.79	0.47	
2:A:950:ARG:NH1	2:A:951:SER:O	2.48	0.47	
1:B:411:GLN:HB2	1:B:418:ARG:HB3	1.97	0.47	
2:A:729:LEU:HD12	2:A:729:LEU:HA	1.77	0.47	
2:A:868:THR:HG22	2:A:910:GLY:HA3	1.97	0.47	
1:B:326:ASP:OD1	1:B:327:TYR:N	2.45	0.47	
2:A:387:ILE:HG23	2:A:389:MET:SD	2.55	0.47	
2:A:829:CYS:HB2	2:A:866:TYR:CE2	2.50	0.47	
2:A:452:ASP:OD1	2:A:452:ASP:N	2.48	0.46	
1:B:448:CYS:HA	1:B:472:THR:HG21	1.98	0.46	
1:B:199:LYS:NZ	1:B:263:ASP:OD2	2.41	0.46	
2:A:869:SER:HB2	2:A:944:THR:HB	1.97	0.46	
2:A:350:THR:OG1	2:A:353:GLU:OE1	2.31	0.46	
2:A:874:TYR:CE1	2:A:903:LEU:HG	2.50	0.46	
1:B:144:PHE:HB3	1:B:437:VAL:HG22	1.97	0.46	
2:A:885:LYS:NZ	2:A:893:CYS:HB3	2.30	0.45	



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		Interatomic	Clash		
Atom-1	Atom-2	distance (Å)	overlap (Å)		
1:B:449:LEU:HB2	1:B:472:THR:OG1	2.16	0.45		
2:A:67:LEU:HD13	2:A:97:VAL:HG21	1.98	0.45		
2:A:326:ILE:HD11	2:A:336:ARG:HH22	1.81	0.45		
2:A:881:LYS:H	2:A:881:LYS:HD3	1.81	0.45		
2:A:154:VAL:HG12	2:A:156:THR:HG23	1.97	0.45		
2:A:656:SER:OG	2:A:658:ASP:OD1	2.35	0.45		
2:A:753:ARG:NH2	2:A:763:GLU:OE2	2.50	0.45		
2:A:151:ASP:OD1	2:A:497:ARG:NH1	2.50	0.45		
2:A:20:ASN:HD21	2:A:588:SER:HA	1.82	0.45		
1:B:484:GLN:HG3	1:B:494:HIS:CD2	2.52	0.45		
2:A:330:LYS:HB3	2:A:331:MET:HE1	1.98	0.45		
2:A:935:ARG:NE	2:A:935:ARG:H	2.14	0.45		
1:B:208:VAL:HB	1:B:211:LYS:HB2	1.98	0.45		
1:B:297:ASP:OD2	2:A:482:ARG:NH1	2.50	0.44		
1:B:488:CYS:HB3	1:B:500:CYS:HB3	1.43	0.44		
1:B:343:GLN:HG2	1:B:365:LYS:HB3	1.99	0.44		
2:A:490:PHE:HB3	2:A:501:PHE:HB3	1.99	0.44		
1:B:125:PRO:O	1:B:466:LEU:HD23	2.17	0.44		
2:A:883:MET:HE1	2:A:885:LYS:HE2	1.99	0.44		
2:A:576:ARG:HD2	2:A:601:LEU:HD13	1.98	0.44		
2:A:842:GLN:OE1	2:A:960:GLN:N	2.49	0.44		
2:A:845:VAL:HG12	2:A:846:VAL:N	2.33	0.44		
1:B:495:LEU:HA	1:B:501:SER:H	1.82	0.44		
2:A:719:GLY:HA2	2:A:803:PRO:HD3	1.99	0.44		
2:A:389:MET:SD	2:A:389:MET:N	2.91	0.43		
2:A:846:VAL:O	2:A:848:LEU:HD22	2.18	0.43		
1:B:523:LEU:HD12	1:B:524:GLU:N	2.32	0.43		
2:A:705:LEU:HD11	2:A:787:VAL:HG21	1.99	0.43		
2:A:217:ASP:HA	2:A:220:ARG:HE	1.83	0.43		
2:A:881:LYS:HD2	2:A:926:GLN:HB3	1.99	0.43		
2:A:153:ARG:HH22	2:A:158:ASP:HB2	1.82	0.43		
1:B:153:ASP:OD2	1:B:278:ARG:HG2	2.19	0.43		
1:B:295:ALA:HB2	1:B:329:SER:HB3	2.00	0.43		
2:A:253:GLU:OE2	2:A:268:ARG:NH1	2.52	0.43		
2:A:839:VAL:HG11	2:A:957:HIS:HB3	2.00	0.43		
1:B:266:LEU:HD22	1:B:328:PRO:HB3	2.00	0.43		
1:B:502:CYS:SG	1:B:507:LEU:HA	2.59	0.43		
1:B:56:LEU:HD11	1:B:474:CYS:HB2	2.00	0.43		
1:B:507:LEU:HD13	1:B:508:GLY:N	2.34	0.43		
1:B:82:ARG:HB2	1:B:85:GLU:OE1	2.19	0.42		
1:B:245:GLU:OE2	1:B:248:ARG:NH2	2.51	0.42		



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	lous page	Interatomic	Clash
Atom-1	Atom-2	distance (Å)	overlap (Å)
2:A:307:MET:O	2:A:337:PHE:N	2.51	0.42
2:A:148:LEU:HD23	2:A:148:LEU:HA	1.89	0.42
2:A:962:ARG:O	2:A:962:ARG:NH1	2.52	0.42
1:B:105:VAL:HA	1:B:128:VAL:HG23	2.00	0.42
2:A:114:ARG:HD3	2:A:114:ARG:HA	1.86	0.42
2:A:621:HIS:N	2:A:624:GLY:O	2.41	0.42
1:B:547:ARG:HG2	1:B:548:CYS:H	1.84	0.42
2:A:40:SER:HB3	2:A:55:VAL:HG12	2.02	0.42
2:A:213:ILE:HG23	2:A:217:ASP:HB3	2.00	0.42
2:A:630:SER:OG	2:A:808:TYR:OH	2.32	0.42
2:A:720:LEU:HB3	2:A:755:TRP:HB3	2.00	0.42
1:B:365:LYS:HA	1:B:365:LYS:HD2	1.81	0.42
1:B:544:GLN:HE21	1:B:547:ARG:HB3	1.85	0.42
2:A:944:THR:HA	2:A:950:ARG:NH1	2.34	0.42
1:B:151:PRO:HB2	1:B:280:VAL:HG11	2.02	0.42
2:A:339:ILE:HD12	2:A:378:LEU:HD11	2.02	0.41
1:B:157:LEU:HD11	1:B:264:ALA:HB1	2.01	0.41
1:B:239:ALA:O	1:B:243:GLU:HG2	2.20	0.41
2:A:870:MET:O	2:A:906:ASN:HA	2.20	0.41
1:B:404:VAL:HA	1:B:444:GLN:O	2.21	0.41
2:A:256:LEU:HD11	2:A:299:SER:HA	2.03	0.41
2:A:248:GLY:HA3	2:A:277:SER:HB2	2.02	0.41
2:A:345:PHE:O	2:A:351:ALA:HB2	2.20	0.41
2:A:908:ARG:HH12	2:A:911:HIS:HB2	1.86	0.41
1:B:63:TRP:HZ2	1:B:499:VAL:HB	1.85	0.41
1:B:282:ARG:NH1	1:B:340:ALA:O	2.53	0.41
1:B:328:PRO:HB2	1:B:333:VAL:HG23	2.03	0.41
2:A:424:PHE:CZ	3:C:1:NAG:H61	2.56	0.41
2:A:525:MET:HE1	2:A:586:ASP:HB2	2.03	0.41
2:A:306:VAL:HA	2:A:335:GLU:HB3	2.02	0.41
2:A:777:GLU:H	2:A:777:GLU:HG3	1.63	0.41
2:A:725:LEU:HD12	2:A:790:GLN:O	2.21	0.41
2:A:214:ASP:HB2	2:A:216:PRO:HD2	2.02	0.40
2:A:222:LYS:HE2	2:A:272:ILE:HG12	2.03	0.40
2:A:714:THR:OG1	2:A:715:ALA:N	2.55	0.40
2:A:866:TYR:HB3	2:A:867:MET:CE	2.52	0.40
1:B:67:LEU:HD22	1:B:487:HIS:CD2	2.57	0.40
2:A:54:LEU:HA	2:A:68:HIS:O	2.21	0.40
2:A:829:CYS:HB3	2:A:864:ASP:HB2	2.04	0.40
2:A:845:VAL:HB	2:A:846:VAL:HG23	2.03	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	Perce	ntiles
1	В	506/826~(61%)	470 (93%)	36 (7%)	0	100	100
2	А	905/1198~(76%)	840 (93%)	65~(7%)	0	100	100
All	All	1411/2024~(70%)	1310 (93%)	101 (7%)	0	100	100

There are no Ramachandran outliers to report.

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	В	435/695~(63%)	421 (97%)	14 (3%)	39 68
2	А	765/1021~(75%)	720 (94%)	45~(6%)	19 43
All	All	1200/1716~(70%)	1141 (95%)	59 (5%)	29 52

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	В	91	CYS
1	В	128	VAL
1	В	139	GLN
1	В	166	ASP
1	В	274	GLN
1	В	290	ASP
1	В	294	THR
1	В	321	ARG



Mol	Chain	Res	Type
1	В	429	ASN
1	В	506	ARG
1	В	507	LEU
1	В	527	CYS
1	В	543	CYS
1	В	544	GLN
2	А	19	PHE
2	А	75	ASP
2	А	89	LYS
2	А	99	ARG
2	А	113	ARG
2	А	121	GLU
2	А	136	GLN
2	A	220	ARG
2	А	228	MET
2	А	236	CYS
2	А	239	CYS
2	А	249	VAL
2	А	253	GLU
2	А	271	ASN
2	А	285	MET
2	А	310	LEU
2	А	330	LYS
2	А	331	MET
2	А	336	ARG
2	А	349	ARG
2	А	378	LEU
2	А	421	VAL
2	А	486	HIS
2	А	513	TYR
2	А	516	SER
2	A	517	GLU
2	А	623	ASP
2	А	662	ASP
2	A	681	ARG
2	A	720	LEU
2	А	745	VAL
2	A	759	SER
2	A	773	GLU
2	A	777	GLU
2	A	798	THR
2	А	816	GLN



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Mol	Chain	\mathbf{Res}	Type					
2	А	867	MET					
2	А	870	MET					
2	А	878	LEU					
2	А	883	MET					
2	А	903	LEU					
2	А	923	VAL					
2	А	925	TRP					
2	А	935	ARG					
2	А	950	ARG					

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	В	444	GLN
1	В	471	HIS
2	А	231	ASN
2	А	251	GLN

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)

3 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	Tuno	Chain	Dec Link		Bo	ond leng	ths	В	ond ang	les
WIOI	Type	Ullalli	nes		Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	NAG	С	1	2,3	14,14,15	0.33	0	$17,\!19,\!21$	0.38	0



Mal	Turne	Chain	Dec	Tiple	Bo	ond leng	$_{\rm ths}$	B	ond ang	les
IVIOI	туре	Chain	nes	LINK	Counts	RMSZ	# Z >2	Counts	RMSZ	# Z > 2
3	NAG	С	2	3	14,14,15	0.21	0	17,19,21	0.43	0
3	BMA	С	3	3	11,11,12	0.58	0	15,15,17	0.70	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	С	1	NAG	1	0

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





5.6 Ligand geometry (i)

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

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-60143. 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



6.1.2 Raw map



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



6.2 Central slices (i)

6.2.1 Primary map



X Index: 105



Y Index: 105



Z Index: 105

6.2.2 Raw map



X Index: 105

Y Index: 105

Z Index: 105

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: 101



Y Index: 112



Z Index: 82

6.3.2 Raw map



X Index: 101

Y Index: 110



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



6.4.2 Raw map



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

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.



Mask visualisation (i) 6.6

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

emd_60143_msk_1.map (i) 6.6.1



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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 237 $\rm nm^3;$ this corresponds to an approximate mass of 214 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 0.370 ${\rm \AA^{-1}}$



8 Fourier-Shell correlation (i)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC (i)



*Reported resolution corresponds to spatial frequency of 0.370 ${\rm \AA^{-1}}$



8.2 Resolution estimates (i)

$\begin{bmatrix} Bosolution ostimato (Å) \end{bmatrix}$	Estimation criterion		criterion (FSC cut-off)
resolution estimate (A)	0.143	0.5	Half-bit
Reported by author	2.70	-	-
Author-provided FSC curve	2.70	2.96	2.74
Unmasked-calculated*	3.11	3.44	3.15

*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 3.11 differs from the reported value 2.7 by more than 10 %



9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-60143 and PDB model 8ZJF. 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 0.012 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 (0.012).



9.4 Atom inclusion (i)



At the recommended contour level, 97% of all backbone atoms, 96% 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 (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9580	0.4150
А	0.9540	0.3970
В	0.9670	0.4460
С	0.9490	0.4890



