Full wwPDB EM Validation Report

Mar 15, 2025 – 09:02 pm GMT

PDB ID	:	8REW
EMDB ID	:	EMD-19110
Title	:	CryoEM structure of human GARP-lTGFbeta1 in complex with a Fab fragment derived from an activating antibody.
Authors	:	Felix, J.; Lambert, F.; Marien, L.; van der Woning, B.; Savvides, S.N.; Lucas, S.
Deposited on	:	2023-12-12
Resolution	:	2.98 Å(reported)
Based on initial model	:	6GFF

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:

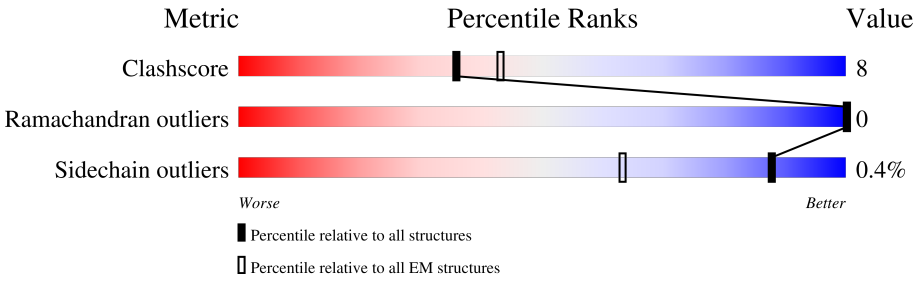
EMDB validation analysis	:	FAILED
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

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 2.98 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Mol	Chain	Length	Quality of chain
1	A	390	44% 10% 46%
1	B	390	21% 6% 73%
1	C	390	43% 10% 47%
1	D	390	24% · 73%
2	E	674	62% 14% 24%
3	F	238	39% 8% 53%
3	I	238	39% 8% 52%
4	G	247	36% 12% 51%
4	H	247	41% 9% 50%

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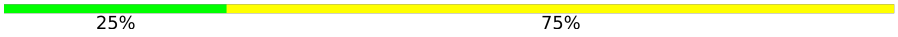
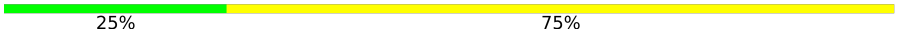
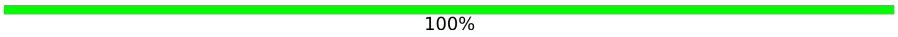
Mol	Chain	Length	Quality of chain
5	J	4	
5	K	4	
6	L	2	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 12428 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 Transforming growth factor beta-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	210	Total	C	N	O	S	0	0
			1642	1044	292	299	7		
1	B	104	Total	C	N	O	S	0	0
			815	525	136	144	10		
1	C	208	Total	C	N	O	S	0	0
			1649	1046	292	304	7		
1	D	107	Total	C	N	O	S	0	0
			815	523	136	146	10		

- Molecule 2 is a protein called Transforming growth factor beta activator LRRC32.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	E	510	Total	C	N	O	S	0	0
			3795	2417	647	717	14		

There are 46 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	629	GLU	-	expression tag	UNP Q14392
E	630	ALA	-	expression tag	UNP Q14392
E	631	ALA	-	expression tag	UNP Q14392
E	632	ALA	-	expression tag	UNP Q14392
E	633	GLU	-	expression tag	UNP Q14392
E	634	ASN	-	expression tag	UNP Q14392
E	635	LEU	-	expression tag	UNP Q14392
E	636	TYR	-	expression tag	UNP Q14392
E	637	PHE	-	expression tag	UNP Q14392
E	638	GLN	-	expression tag	UNP Q14392
E	639	GLY	-	expression tag	UNP Q14392
E	640	ALA	-	expression tag	UNP Q14392
E	641	ALA	-	expression tag	UNP Q14392
E	642	TRP	-	expression tag	UNP Q14392
E	643	SER	-	expression tag	UNP Q14392

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Chain	Residue	Modelled	Actual	Comment	Reference
E	644	HIS	-	expression tag	UNP Q14392
E	645	PRO	-	expression tag	UNP Q14392
E	646	GLN	-	expression tag	UNP Q14392
E	647	PHE	-	expression tag	UNP Q14392
E	648	GLU	-	expression tag	UNP Q14392
E	649	LYS	-	expression tag	UNP Q14392
E	650	GLY	-	expression tag	UNP Q14392
E	651	ALA	-	expression tag	UNP Q14392
E	652	ALA	-	expression tag	UNP Q14392
E	653	TRP	-	expression tag	UNP Q14392
E	654	SER	-	expression tag	UNP Q14392
E	655	HIS	-	expression tag	UNP Q14392
E	656	PRO	-	expression tag	UNP Q14392
E	657	GLN	-	expression tag	UNP Q14392
E	658	PHE	-	expression tag	UNP Q14392
E	659	GLU	-	expression tag	UNP Q14392
E	660	LYS	-	expression tag	UNP Q14392
E	661	GLY	-	expression tag	UNP Q14392
E	662	ALA	-	expression tag	UNP Q14392
E	663	ALA	-	expression tag	UNP Q14392
E	664	TRP	-	expression tag	UNP Q14392
E	665	SER	-	expression tag	UNP Q14392
E	666	HIS	-	expression tag	UNP Q14392
E	667	PRO	-	expression tag	UNP Q14392
E	668	GLN	-	expression tag	UNP Q14392
E	669	PHE	-	expression tag	UNP Q14392
E	670	GLU	-	expression tag	UNP Q14392
E	671	LYS	-	expression tag	UNP Q14392
E	672	GLY	-	expression tag	UNP Q14392
E	673	ALA	-	expression tag	UNP Q14392
E	674	ALA	-	expression tag	UNP Q14392

- Molecule 3 is a protein called hFab LHT-22, Light Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	F	112	Total	C	N	O	S	0	0
			822	513	142	164	3		
3	I	114	Total	C	N	O	S	0	0
			835	520	145	167	3		

- Molecule 4 is a protein called hFab LHT-22, Heavy Chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	120	Total	C	N	O	S	0	0
			911	574	152	179	6		
4	H	124	Total	C	N	O	S	0	0
			946	595	158	187	6		

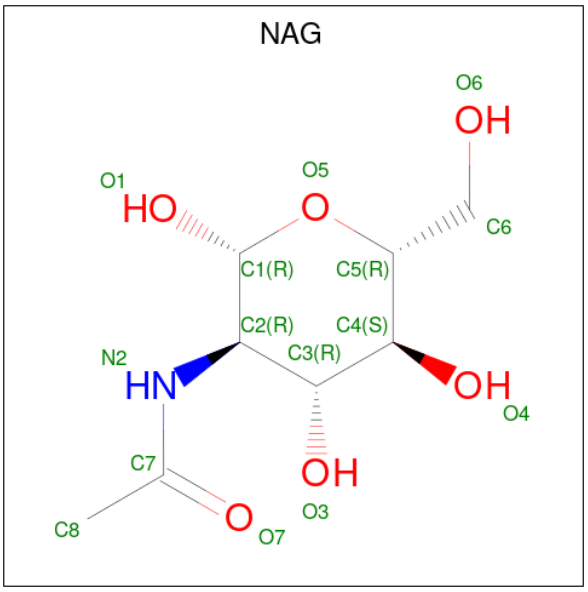
- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms				AltConf	Trace
5	J	4	Total	C	N	O	0	0
			50	28	2	20		
5	K	4	Total	C	N	O	0	0
			50	28	2	20		

- Molecule 6 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
6	L	2	Total	C	N	O	0	0
			28	16	2	10		

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



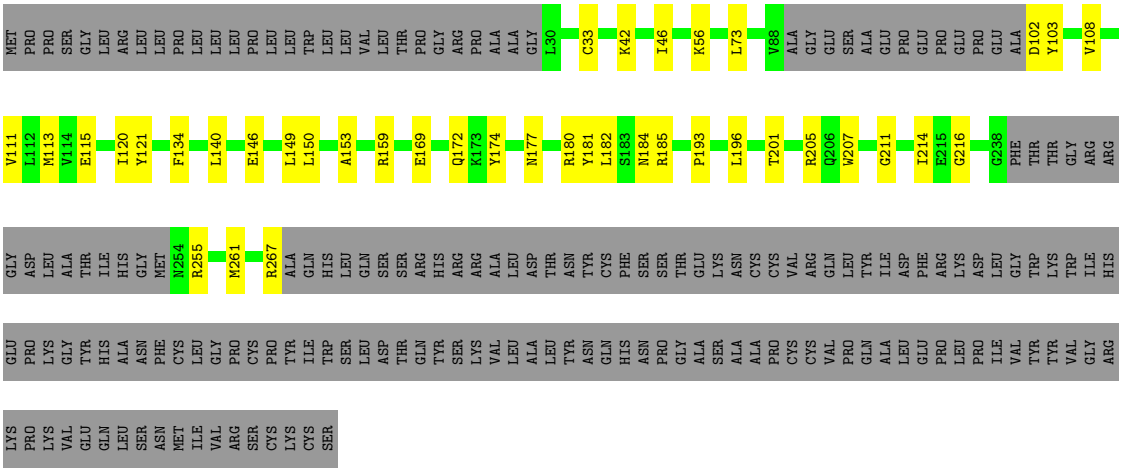
Mol	Chain	Residues	Atoms				AltConf
7	A	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	C	1	Total	C	N	O	0
			14	8	1	5	
7	E	1	Total	C	N	O	0
			14	8	1	5	
7	E	1	Total	C	N	O	0
			14	8	1	5	

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. 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. 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.

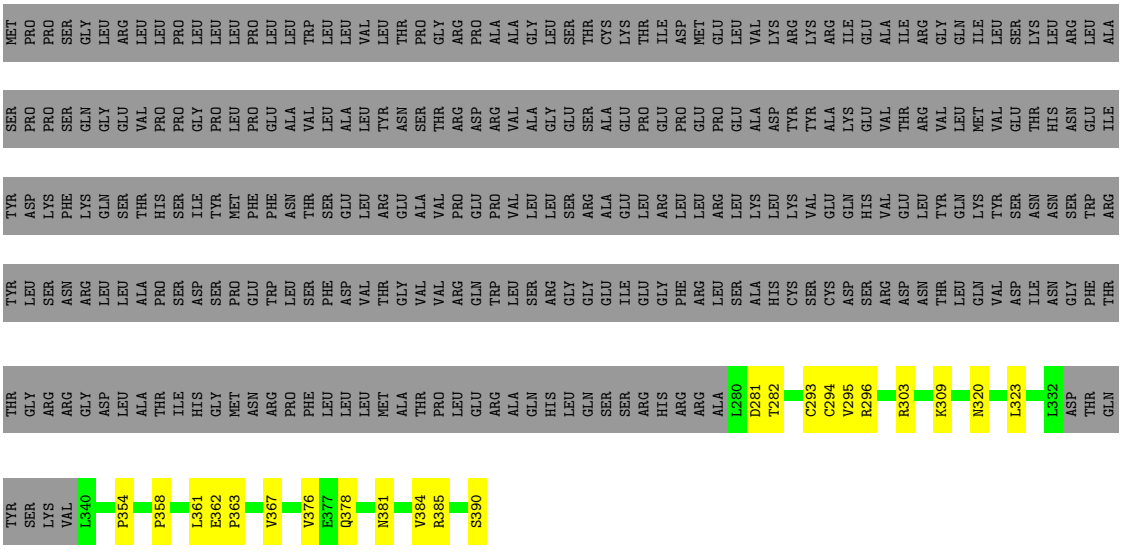
• Molecule 1: Transforming growth factor beta-1

Chain A:



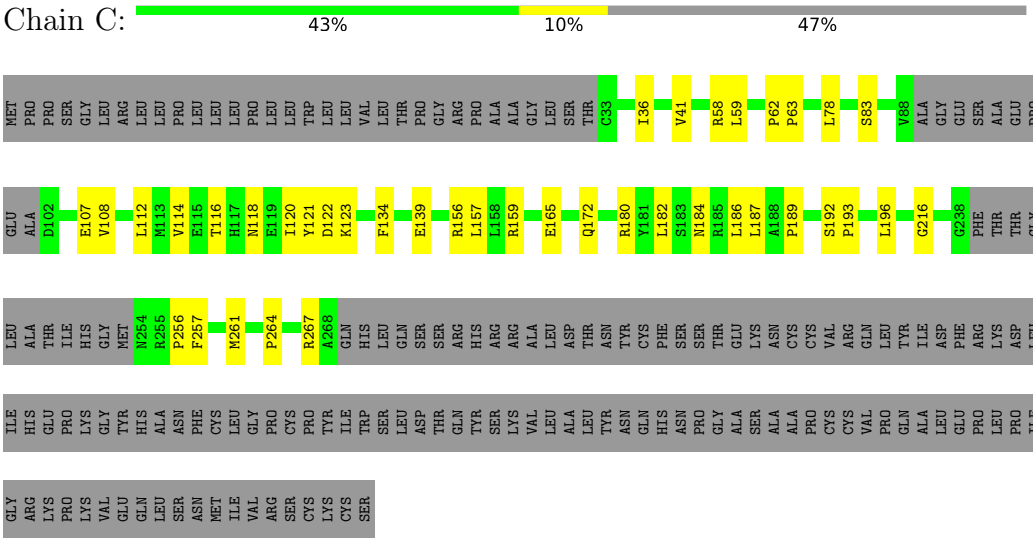
• Molecule 1: Transforming growth factor beta-1

Chain B:



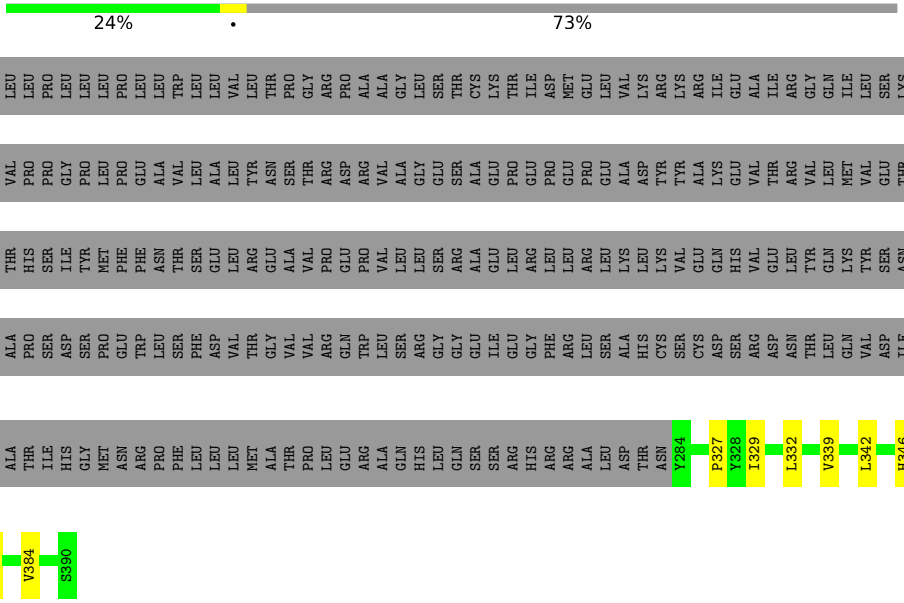
• Molecule 1: Transforming growth factor beta-1

Chain C:



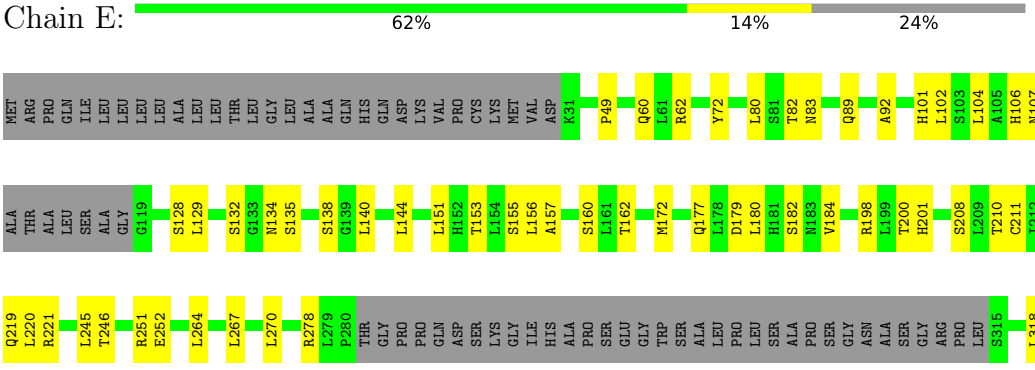
• Molecule 1: Transforming growth factor beta-1

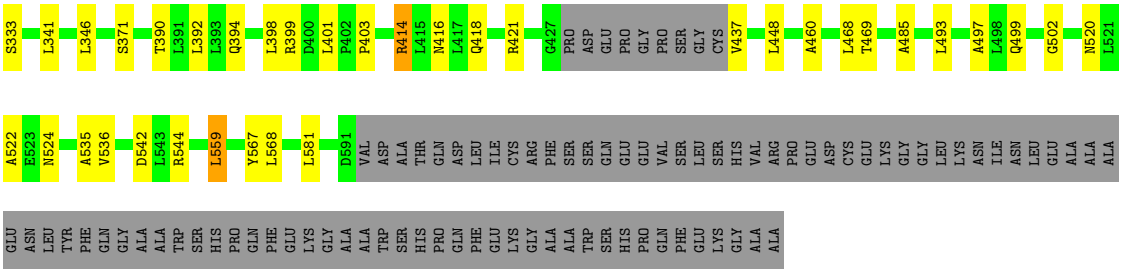
Chain D:



• Molecule 2: Transforming growth factor beta activator LRRC32

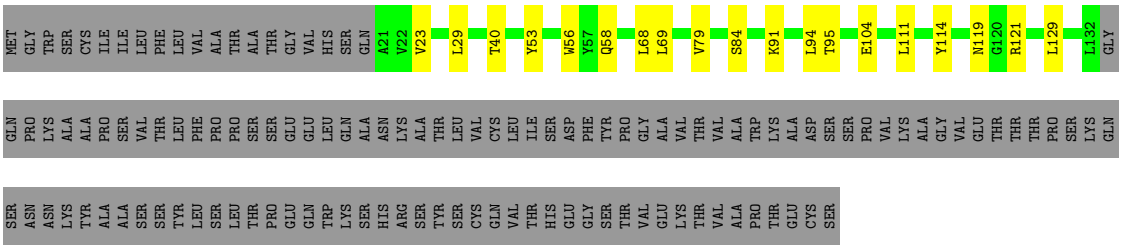
Chain E:





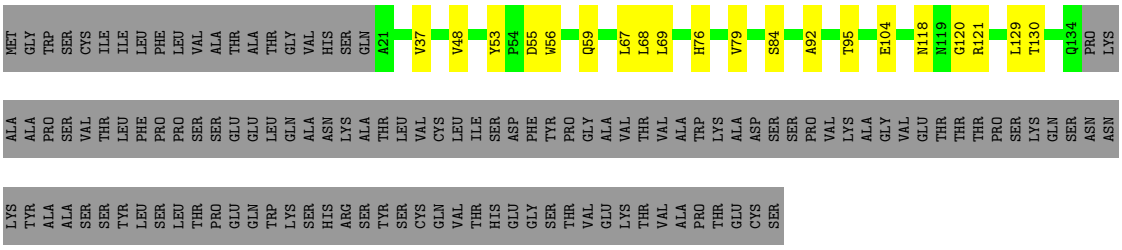
• Molecule 3: hFab LHT-22, Light Chain

Chain F:



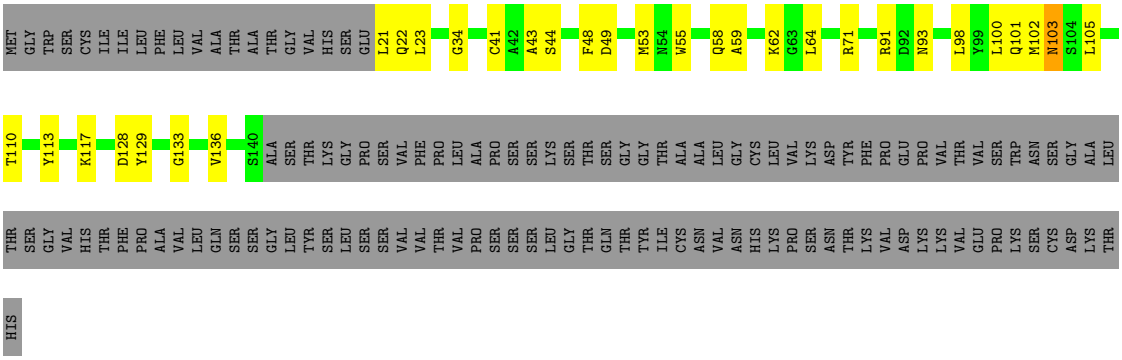
• Molecule 3: hFab LHT-22, Light Chain

Chain I:



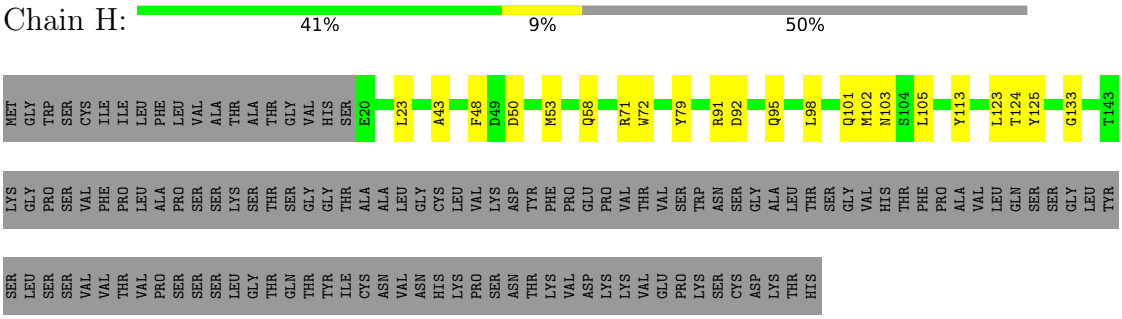
• Molecule 4: hFab LHT-22, Heavy Chain

Chain G:



• Molecule 4: hFab LHT-22, Heavy Chain

Chain H:

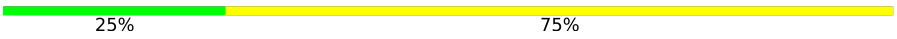


• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

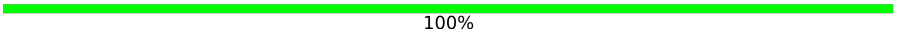
• Molecule 5: alpha-D-mannopyranose-(1-6)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:



• Molecule 6: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	320551	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	JEOL CRYO ARM 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	61.8	Depositor
Minimum defocus (nm)	800	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.32	0/1675	0.60	0/2277
1	B	0.33	0/841	0.54	0/1149
1	C	0.28	0/1682	0.55	0/2282
1	D	0.27	0/841	0.50	0/1153
2	E	0.26	0/3857	0.54	2/5257 (0.0%)
3	F	0.30	0/840	0.57	0/1148
3	I	0.30	0/853	0.58	0/1165
4	G	0.29	0/931	0.58	0/1264
4	H	0.29	0/966	0.60	0/1309
All	All	0.29	0/12486	0.56	2/17004 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	559	LEU	CA-CB-CG	5.79	128.61	115.30
2	E	346	LEU	CA-CB-CG	5.12	127.07	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1642	0	1609	27	0
1	B	815	0	763	17	0
1	C	1649	0	1627	29	0
1	D	815	0	751	12	0
2	E	3795	0	3749	54	0
3	F	822	0	796	11	0
3	I	835	0	807	13	0
4	G	911	0	859	22	0
4	H	946	0	904	18	0
5	J	50	0	43	2	0
5	K	50	0	43	1	0
6	L	28	0	25	0	0
7	A	14	0	13	0	0
7	C	28	0	26	0	0
7	E	28	0	26	0	0
All	All	12428	0	12041	187	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (187) 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:D:342:LEU:O	1:D:346:HIS:HB2	1.65	0.97
1:A:56:LYS:NZ	1:D:380:SER:O	2.23	0.72
4:H:113:TYR:O	4:H:133:GLY:HA2	1.90	0.71
1:D:339:VAL:HG21	2:E:160:SER:HB3	1.72	0.71
3:I:104:GLU:HG3	3:I:130:THR:HA	1.74	0.70
1:A:108:VAL:HG22	1:A:261:MET:HG3	1.75	0.69
1:C:116:THR:HA	1:C:121:TYR:CD2	2.28	0.68
1:C:134:PHE:HD1	1:C:216:GLY:HA3	1.58	0.68
1:B:363:PRO:HB3	1:B:378:GLN:HE21	1.59	0.68
4:H:48:PHE:HB3	4:H:91:ARG:HH21	1.58	0.68
1:D:327:PRO:HB2	2:E:208:SER:HB3	1.76	0.67
4:H:79:TYR:H	3:I:118:ASN:HD21	1.40	0.67
1:C:157:LEU:HD23	1:C:256:PRO:HB3	1.77	0.67
3:F:53:TYR:O	3:F:121:ARG:NH1	2.27	0.67
1:B:303:ARG:HD2	1:B:309:LYS:HE3	1.76	0.67
1:C:108:VAL:HG22	1:C:261:MET:HG2	1.78	0.65
2:E:499:GLN:HG3	2:E:522:ALA:HB3	1.79	0.63
3:F:104:GLU:HA	3:F:129:LEU:O	1.98	0.63
1:A:120:ILE:HG12	1:A:214:ILE:HG21	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:116:THR:HA	1:C:121:TYR:CE2	2.34	0.63
3:F:40:THR:HG22	3:F:91:LYS:HE2	1.81	0.63
4:G:113:TYR:O	4:G:133:GLY:HA2	1.99	0.62
1:B:294:CYS:SG	1:B:296:ARG:NH1	2.73	0.62
1:C:187:LEU:HD21	1:C:196:LEU:HD11	1.81	0.62
1:A:174:TYR:OH	1:A:180:ARG:NH1	2.33	0.62
1:C:157:LEU:HB2	1:C:196:LEU:HB2	1.81	0.61
2:E:101:HIS:HA	2:E:128:SER:HB3	1.81	0.61
4:G:21:LEU:HA	4:G:44:SER:O	2.01	0.61
1:A:159:ARG:O	1:A:193:PRO:HA	2.01	0.60
1:C:83:SER:O	1:C:156:ARG:NH2	2.30	0.60
4:H:124:THR:HG22	4:H:125:TYR:H	1.66	0.60
3:F:58:GLN:HB2	3:F:68:LEU:HD11	1.83	0.60
4:G:34:GLY:N	4:G:105:LEU:O	2.35	0.59
2:E:544:ARG:HH12	2:E:567:TYR:HB3	1.67	0.59
1:B:282:THR:HG22	1:B:295:VAL:HG11	1.84	0.58
4:G:58:GLN:HB2	4:G:64:LEU:HD23	1.84	0.58
1:C:114:VAL:HG11	1:C:120:ILE:HD11	1.86	0.58
1:A:102:ASP:OD1	1:A:103:TYR:N	2.37	0.58
1:C:107:GLU:HB2	1:C:264:PRO:HG3	1.86	0.57
3:F:56:TRP:HB2	3:F:69:LEU:HB2	1.86	0.57
4:G:41:CYS:HB3	4:G:98:LEU:HB3	1.86	0.57
1:C:123:LYS:HE3	4:H:50:ASP:HA	1.86	0.57
1:D:367:VAL:HG22	1:D:376:VAL:HG22	1.86	0.56
1:A:150:LEU:O	1:A:205:ARG:NH1	2.39	0.56
2:E:390:THR:HG23	2:E:414:ARG:HD2	1.87	0.56
1:A:113:MET:SD	1:A:121:TYR:OH	2.59	0.56
4:H:23:LEU:HD23	4:H:43:ALA:HB2	1.88	0.55
1:B:367:VAL:HG22	1:B:376:VAL:HG22	1.87	0.55
2:E:460:ALA:HA	2:E:485:ALA:HA	1.87	0.55
1:B:354:PRO:HA	1:B:390:SER:O	2.07	0.54
1:C:165:GLU:HB3	1:C:189:PRO:HD3	1.88	0.54
3:I:56:TRP:HB2	3:I:69:LEU:HB2	1.89	0.54
3:I:84:SER:OG	3:I:95:THR:OG1	2.25	0.54
1:A:115:GLU:HG3	1:A:255:ARG:HH12	1.73	0.53
1:C:172:GLN:HB3	1:C:182:LEU:HD11	1.89	0.53
4:H:71:ARG:HH21	4:H:72:TRP:HZ3	1.55	0.53
2:E:49:PRO:HA	2:E:72:TYR:HD1	1.74	0.53
1:B:362:GLU:OE1	1:B:385:ARG:NH2	2.41	0.53
4:G:71:ARG:O	4:G:91:ARG:NH1	2.42	0.53
2:E:107:ASN:N	2:E:134:ASN:OD1	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:67:LEU:HD22	3:I:76:HIS:HB2	1.91	0.52
1:C:112:LEU:HD23	1:C:257:PHE:HB3	1.91	0.52
2:E:403:PRO:HA	2:E:437:VAL:HA	1.91	0.52
2:E:536:VAL:H	2:E:559:LEU:HB3	1.74	0.52
2:E:278:ARG:HG2	2:E:326:GLU:HB3	1.92	0.52
1:D:332:LEU:HD21	2:E:182:SER:HB3	1.90	0.52
1:A:172:GLN:OE1	1:A:180:ARG:NH2	2.42	0.51
2:E:497:ALA:HA	2:E:520:ASN:HB3	1.92	0.51
4:G:34:GLY:CA	4:G:105:LEU:O	2.58	0.51
2:E:469:THR:HA	2:E:493:LEU:HA	1.93	0.51
1:A:169:GLU:HG2	1:A:184:ASN:HD21	1.76	0.51
1:A:267:ARG:NH1	1:D:377:GLU:OE2	2.43	0.51
1:B:361:LEU:HB3	1:B:381:ASN:HA	1.92	0.51
1:B:358:PRO:HB3	1:B:384:VAL:HG13	1.93	0.50
1:A:146:GLU:HB3	1:A:149:LEU:HG	1.92	0.50
1:B:293:CYS:HA	1:B:323:LEU:O	2.11	0.50
2:E:246:THR:HA	2:E:267:LEU:HA	1.94	0.50
3:I:55:ASP:OD2	3:I:121:ARG:NH2	2.45	0.49
1:C:159:ARG:O	1:C:193:PRO:HA	2.12	0.49
4:G:48:PHE:O	4:G:91:ARG:NH2	2.46	0.49
2:E:49:PRO:HA	2:E:72:TYR:CD1	2.48	0.49
3:F:69:LEU:HD12	3:F:94:LEU:HD12	1.94	0.48
2:E:245:LEU:HB3	2:E:264:LEU:HD22	1.95	0.48
1:A:42:LYS:O	1:A:46:ILE:HG12	2.14	0.48
4:H:113:TYR:O	4:H:133:GLY:CA	2.61	0.48
2:E:198:ARG:HA	2:E:219:GLN:HG2	1.96	0.48
2:E:371:SER:HB2	2:E:394:GLN:HG2	1.96	0.48
2:E:60:GLN:O	2:E:62:ARG:NH1	2.43	0.48
2:E:392:LEU:HA	2:E:416:ASN:HB3	1.95	0.48
3:I:68:LEU:HA	3:I:79:VAL:HG21	1.95	0.48
2:E:80:LEU:O	2:E:83:ASN:ND2	2.47	0.47
1:D:339:VAL:HG13	1:D:342:LEU:HD12	1.96	0.47
2:E:332:ASP:OD1	2:E:333:SER:N	2.47	0.47
4:H:58:GLN:OE1	3:I:59:GLN:NE2	2.39	0.47
1:A:172:GLN:HB2	1:A:182:LEU:HD11	1.95	0.47
1:D:363:PRO:HB3	1:D:380:SER:HA	1.96	0.47
2:E:153:THR:HA	2:E:177:GLN:HB2	1.96	0.47
4:G:117:LYS:NZ	4:G:128:ASP:OD2	2.44	0.47
1:A:169:GLU:HG2	1:A:184:ASN:ND2	2.29	0.47
1:B:296:ARG:HD3	1:B:323:LEU:HB3	1.96	0.47
1:B:363:PRO:HB3	1:B:378:GLN:NE2	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:101:GLN:OE1	4:H:103:ASN:ND2	2.45	0.47
1:C:58:ARG:HB2	1:C:267:ARG:HD2	1.95	0.46
1:A:184:ASN:OD1	1:C:184:ASN:ND2	2.48	0.46
4:G:22:GLN:HA	4:G:129:TYR:HE2	1.80	0.46
3:F:84:SER:OG	3:F:95:THR:OG1	2.33	0.46
4:H:53:MET:HB3	4:H:98:LEU:HD22	1.96	0.46
1:A:181:TYR:CD2	1:C:186:LEU:HD11	2.51	0.46
2:E:251:ARG:HG3	2:E:252:GLU:HG3	1.97	0.46
2:E:568:LEU:HD22	2:E:581:LEU:HD21	1.97	0.46
3:I:48:VAL:HG11	3:I:92:ALA:HB2	1.97	0.46
4:G:103:ASN:HD22	4:G:103:ASN:C	2.18	0.46
1:C:172:GLN:NE2	1:C:180:ARG:HH21	2.13	0.46
2:E:138:SER:HB2	2:E:162:THR:H	1.81	0.46
4:G:48:PHE:HB3	4:G:91:ARG:HH21	1.81	0.46
4:G:59:ALA:HB3	4:G:62:LYS:HB2	1.99	0.45
4:H:123:LEU:HD21	3:I:120:GLY:HA2	1.97	0.45
3:I:53:TYR:O	3:I:121:ARG:NH2	2.49	0.45
2:E:89:GLN:HB3	2:E:92:ALA:HB2	1.97	0.45
4:G:102:MET:HB3	4:G:105:LEU:HD13	1.99	0.45
2:E:200:THR:HA	2:E:220:LEU:HA	1.98	0.45
4:G:117:LYS:O	4:G:128:ASP:N	2.50	0.45
2:E:217:LEU:HD23	2:E:217:LEU:HA	1.87	0.45
1:A:134:PHE:HA	1:A:216:GLY:HA3	1.98	0.45
4:H:101:GLN:NE2	4:H:103:ASN:OD1	2.45	0.45
1:A:111:VAL:HG11	1:A:140:LEU:HD12	1.99	0.44
2:E:210:THR:OG1	2:E:211:CYS:N	2.49	0.44
4:G:49:ASP:OD1	4:G:93:ASN:ND2	2.39	0.44
2:E:502:GLY:HA2	2:E:524:ASN:HA	1.99	0.44
2:E:267:LEU:HD21	2:E:270:LEU:HB2	1.99	0.44
1:A:153:ALA:HB3	1:A:201:THR:HA	1.98	0.44
1:C:159:ARG:NH2	1:C:192:SER:O	2.48	0.44
1:A:134:PHE:HD1	1:A:216:GLY:HA3	1.82	0.44
2:E:394:GLN:HB3	2:E:418:GLN:HB2	2.00	0.43
1:B:281:ASP:N	1:B:281:ASP:OD1	2.43	0.43
2:E:104:LEU:O	2:E:134:ASN:ND2	2.51	0.43
4:H:92:ASP:HB3	4:H:95:GLN:HB2	2.00	0.43
2:E:520:ASN:HA	2:E:542:ASP:HB2	2.01	0.43
2:E:318:LEU:HA	2:E:341:LEU:HA	2.00	0.43
4:G:23:LEU:HG	4:G:43:ALA:HB2	2.00	0.43
4:G:55:TRP:NE1	4:G:100:LEU:HB2	2.34	0.43
3:F:29:LEU:HD11	3:F:129:LEU:HD12	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:ASP:HB2	4:H:72:TRP:HZ2	1.83	0.43
4:G:117:LYS:HD2	4:G:128:ASP:HB3	1.99	0.43
1:A:33:CYS:HB3	2:E:213:SER:HB2	2.00	0.43
1:B:323:LEU:HD11	1:C:36:ILE:HG12	2.01	0.43
5:J:1:NAG:H61	5:J:2:NAG:HN2	1.81	0.43
1:A:185:ARG:HG2	1:A:196:LEU:HD11	2.01	0.42
1:A:73:LEU:HD23	1:D:367:VAL:HG11	2.01	0.42
1:A:207:TRP:HA	1:A:211:GLY:HA3	2.00	0.42
2:E:151:LEU:HD21	2:E:172:MET:HB2	2.01	0.42
3:F:114:TYR:HA	3:F:119:ASN:HA	2.01	0.42
1:A:115:GLU:HG3	1:A:255:ARG:NH1	2.33	0.42
2:E:156:LEU:HB2	2:E:180:LEU:HD23	2.00	0.42
4:H:102:MET:HB3	4:H:105:LEU:HD21	2.02	0.42
2:E:155:SER:HA	2:E:179:ASP:HB3	2.01	0.42
2:E:82:THR:H	2:E:106:HIS:HB2	1.84	0.42
5:J:1:NAG:H61	5:J:2:NAG:N2	2.35	0.42
1:B:323:LEU:HD13	1:C:41:VAL:HG11	2.02	0.42
1:C:62:PRO:HA	1:C:63:PRO:HD3	1.94	0.42
4:G:53:MET:HB3	4:G:98:LEU:HD11	2.02	0.42
4:H:71:ARG:O	4:H:91:ARG:NH1	2.53	0.42
2:E:102:LEU:HB3	2:E:129:LEU:HD23	2.02	0.41
4:G:34:GLY:HA2	4:G:105:LEU:O	2.19	0.41
1:C:139:GLU:OE2	5:K:1:NAG:O6	2.34	0.41
4:G:110:THR:HA	4:G:136:VAL:O	2.20	0.41
3:I:37:VAL:HG11	3:I:129:LEU:HD11	2.02	0.41
1:D:358:PRO:HB3	1:D:384:VAL:HG13	2.02	0.41
2:E:140:LEU:HD23	2:E:144:LEU:HB2	2.01	0.41
2:E:399:ARG:HD2	2:E:421:ARG:HH22	1.86	0.41
2:E:535:ALA:HA	2:E:559:LEU:H	1.86	0.41
1:B:295:VAL:HG13	1:B:320:ASN:HB3	2.02	0.41
1:C:78:LEU:HD23	1:C:78:LEU:HA	1.92	0.41
1:C:159:ARG:HD3	1:C:187:LEU:HD23	2.03	0.41
4:H:79:TYR:H	3:I:118:ASN:ND2	2.13	0.41
1:B:303:ARG:HD2	1:B:309:LYS:CE	2.49	0.41
1:C:118:ASN:HD22	1:C:118:ASN:HA	1.77	0.41
2:E:110:ALA:HB2	2:E:135:SER:HB3	2.02	0.41
2:E:398:LEU:HD13	2:E:401:LEU:HD11	2.02	0.41
1:C:59:LEU:HD23	1:C:59:LEU:HA	1.92	0.41
3:F:68:LEU:HA	3:F:79:VAL:HG21	2.03	0.41
2:E:132:SER:HA	2:E:157:ALA:O	2.20	0.40
1:D:329:ILE:HG23	2:E:184:VAL:HG13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:448:LEU:HB3	2:E:468:LEU:HD21	2.03	0.40
2:E:109:LEU:HD13	2:E:134:ASN:HD22	1.86	0.40
2:E:200:THR:O	2:E:221:ARG:N	2.42	0.40
3:F:23:VAL:HG22	3:F:111:LEU:HD12	2.02	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	204/390 (52%)	197 (97%)	7 (3%)	0	100	100
1	B	100/390 (26%)	92 (92%)	8 (8%)	0	100	100
1	C	202/390 (52%)	198 (98%)	4 (2%)	0	100	100
1	D	105/390 (27%)	101 (96%)	4 (4%)	0	100	100
2	E	502/674 (74%)	482 (96%)	20 (4%)	0	100	100
3	F	110/238 (46%)	106 (96%)	4 (4%)	0	100	100
3	I	112/238 (47%)	105 (94%)	7 (6%)	0	100	100
4	G	118/247 (48%)	114 (97%)	4 (3%)	0	100	100
4	H	122/247 (49%)	121 (99%)	1 (1%)	0	100	100
All	All	1575/3204 (49%)	1516 (96%)	59 (4%)	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 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	176/346 (51%)	175 (99%)	1 (1%)	84 92
1	B	89/346 (26%)	89 (100%)	0	100 100
1	C	180/346 (52%)	180 (100%)	0	100 100
1	D	87/346 (25%)	87 (100%)	0	100 100
2	E	402/569 (71%)	400 (100%)	2 (0%)	86 94
3	F	89/196 (45%)	89 (100%)	0	100 100
3	I	90/196 (46%)	90 (100%)	0	100 100
4	G	94/205 (46%)	92 (98%)	2 (2%)	48 75
4	H	99/205 (48%)	99 (100%)	0	100 100
All	All	1306/2755 (47%)	1301 (100%)	5 (0%)	88 95

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	ASN
2	E	201	HIS
2	E	414	ARG
4	G	101	GLN
4	G	103	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	233	GLN
1	B	378	GLN
1	C	118	ASN
1	C	172	GLN
3	I	118	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)

10 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	$\#\|Z\| > 2$
5	NAG	J	1	1,5	14,14,15	0.27	0	17,19,21	0.53	0
5	NAG	J	2	5	14,14,15	0.31	0	17,19,21	0.52	0
5	BMA	J	3	5	11,11,12	0.68	0	15,15,17	0.90	0
5	MAN	J	4	5	11,11,12	0.70	0	15,15,17	1.13	2 (13%)
5	NAG	K	1	1,5	14,14,15	0.23	0	17,19,21	0.55	0
5	NAG	K	2	5	14,14,15	0.21	0	17,19,21	0.46	0
5	BMA	K	3	5	11,11,12	1.16	1 (9%)	15,15,17	1.11	1 (6%)
5	MAN	K	4	5	11,11,12	0.72	0	15,15,17	1.07	2 (13%)
6	NAG	L	1	2,6	14,14,15	0.24	0	17,19,21	0.45	0
6	NAG	L	2	6	14,14,15	0.26	0	17,19,21	0.39	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
5	NAG	J	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	J	2	5	-	2/6/23/26	0/1/1/1
5	BMA	J	3	5	-	0/2/19/22	0/1/1/1
5	MAN	J	4	5	-	0/2/19/22	0/1/1/1
5	NAG	K	1	1,5	-	2/6/23/26	0/1/1/1
5	NAG	K	2	5	-	4/6/23/26	0/1/1/1
5	BMA	K	3	5	-	0/2/19/22	0/1/1/1
5	MAN	K	4	5	-	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	L	1	2,6	-	2/6/23/26	0/1/1/1
6	NAG	L	2	6	-	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	K	3	BMA	C2-C3	2.32	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	4	MAN	C1-O5-C5	3.15	116.46	112.19
5	K	3	BMA	C2-C3-C4	2.59	115.37	110.89
5	K	4	MAN	C1-O5-C5	2.27	115.27	112.19
5	K	4	MAN	O2-C2-C3	-2.26	105.61	110.14
5	J	4	MAN	O2-C2-C3	-2.17	105.79	110.14

There are no chirality outliers.

All (14) torsion outliers are listed below:

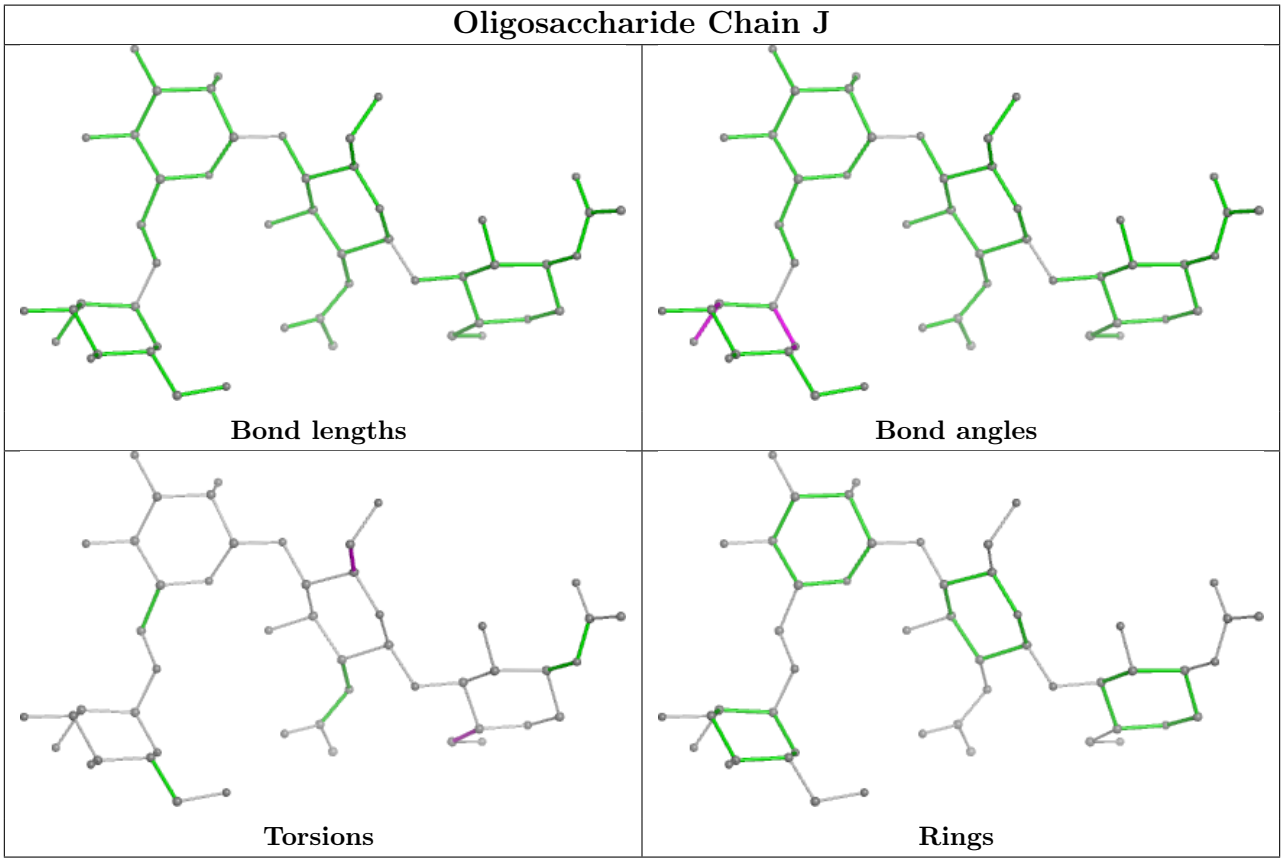
Mol	Chain	Res	Type	Atoms
5	J	1	NAG	O5-C5-C6-O6
6	L	2	NAG	O5-C5-C6-O6
5	J	2	NAG	O5-C5-C6-O6
5	J	2	NAG	C4-C5-C6-O6
5	K	1	NAG	O5-C5-C6-O6
5	J	1	NAG	C4-C5-C6-O6
5	K	1	NAG	C4-C5-C6-O6
5	K	2	NAG	O5-C5-C6-O6
6	L	1	NAG	O5-C5-C6-O6
5	K	2	NAG	C8-C7-N2-C2
5	K	2	NAG	O7-C7-N2-C2
6	L	2	NAG	C4-C5-C6-O6
5	K	2	NAG	C4-C5-C6-O6
6	L	1	NAG	C4-C5-C6-O6

There are no ring outliers.

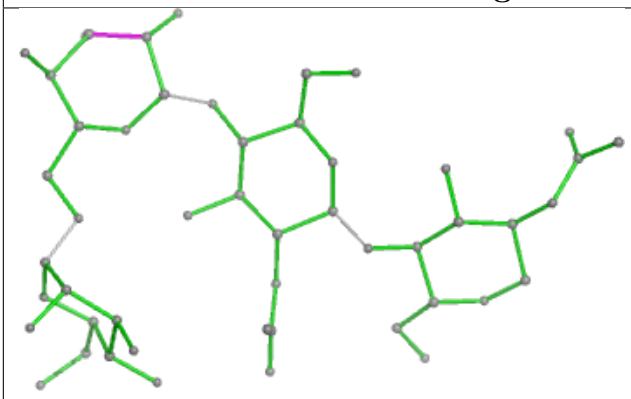
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	K	1	NAG	1	0
5	J	1	NAG	2	0
5	J	2	NAG	2	0

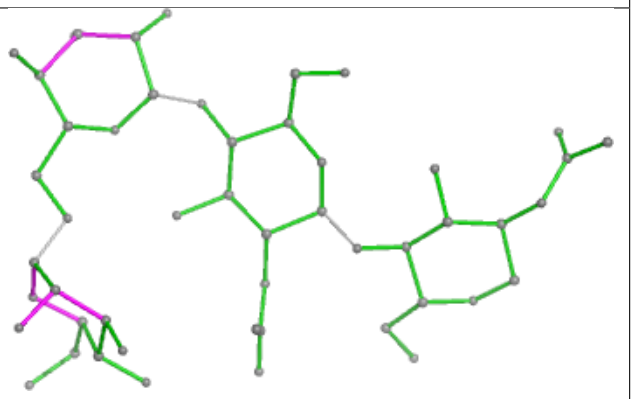
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



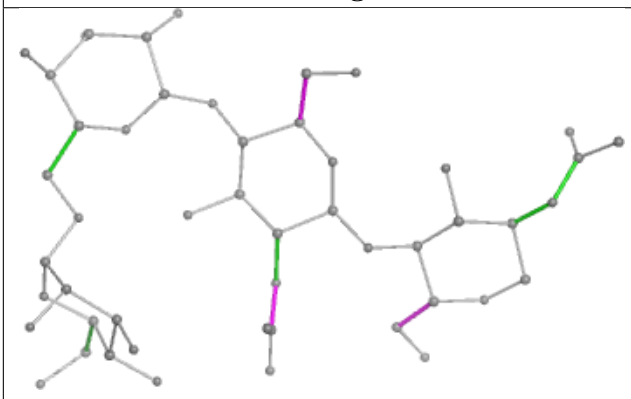
Oligosaccharide Chain K



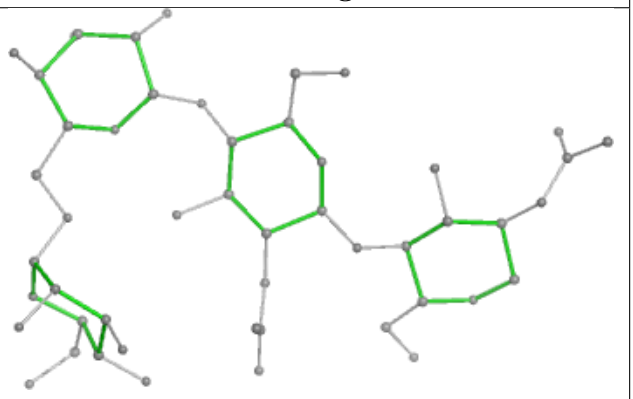
Bond lengths



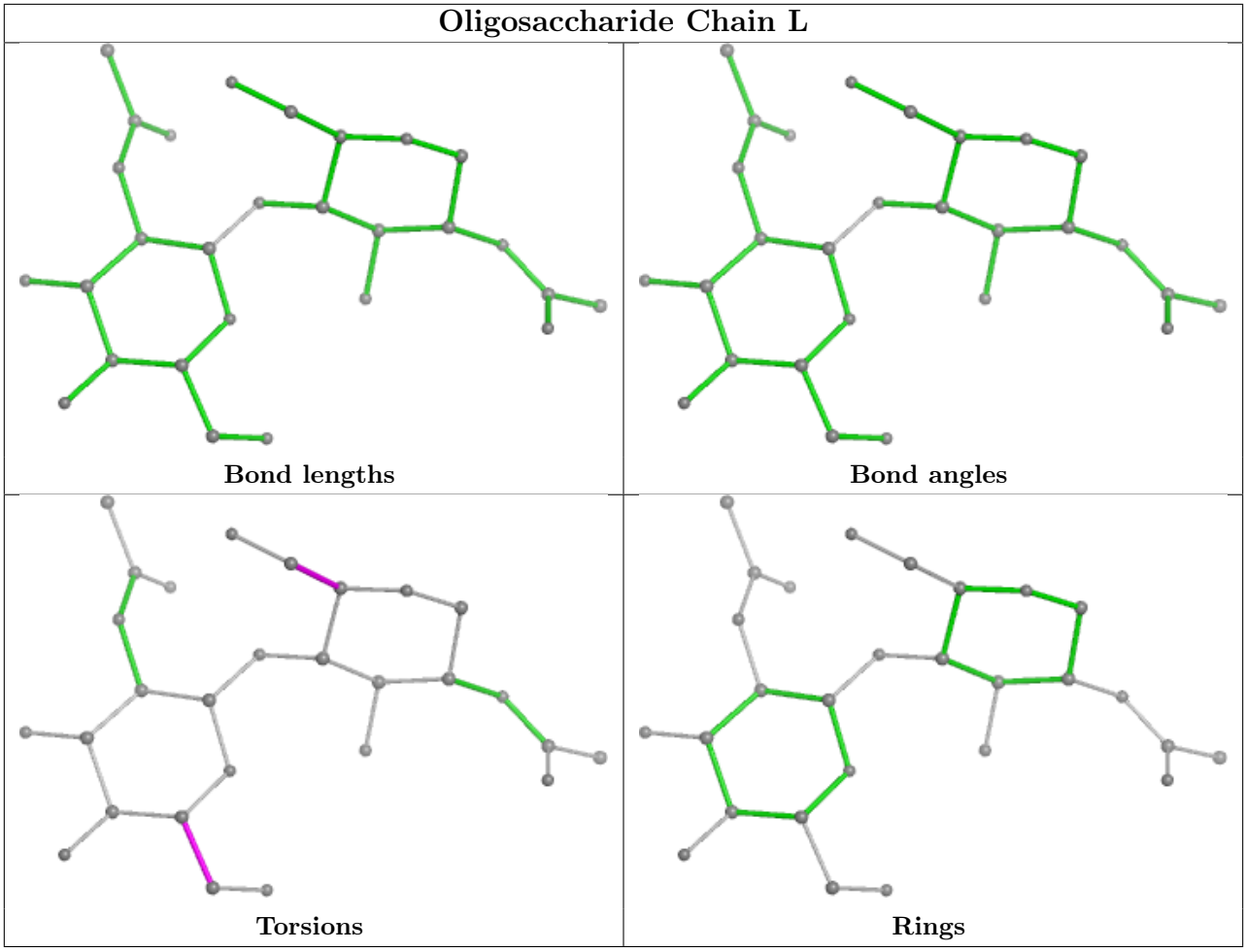
Bond angles



Torsions



Rings



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	$\#\|Z\| > 2$
7	NAG	E	701	2	14,14,15	0.25	0	17,19,21	0.46	0
7	NAG	C	401	1	14,14,15	0.23	0	17,19,21	0.46	0
7	NAG	E	702	2	14,14,15	0.24	0	17,19,21	0.40	0
7	NAG	C	402	1	14,14,15	0.24	0	17,19,21	0.46	0
7	NAG	A	1000	1	14,14,15	0.22	0	17,19,21	0.38	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
7	NAG	E	701	2	-	0/6/23/26	0/1/1/1
7	NAG	C	401	1	-	1/6/23/26	0/1/1/1
7	NAG	E	702	2	-	1/6/23/26	0/1/1/1
7	NAG	C	402	1	-	0/6/23/26	0/1/1/1
7	NAG	A	1000	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	E	702	NAG	O5-C5-C6-O6
7	A	1000	NAG	O5-C5-C6-O6
7	C	401	NAG	O5-C5-C6-O6
7	A	1000	NAG	C4-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.