Full wwPDB EM Validation Report ⓘ

Nov 17, 2022 – 02:09 AM EST

PDB ID	:	7LBF
EMDB ID	:	EMD-23253
Title	:	CryoEM structure of the HCMV Trimer gHgLgO in complex with human Platelet-derived growth factor receptor alpha and neutralizing fabs 13H11 and MSL-109
Authors	:	Kschonsak, M.; Rouge, L.; Arthur, C.P.; Hoangdung, H.; Patel, N.; Kim, I.; Johnson, M.; Kraft, E.; Rohou, A.L.; Gill, A.; Martinez-Martin, N.; Payandeh, J.; Ciferri, C.
Deposited on	:	2021-01-07
Resolution	:	2.80 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

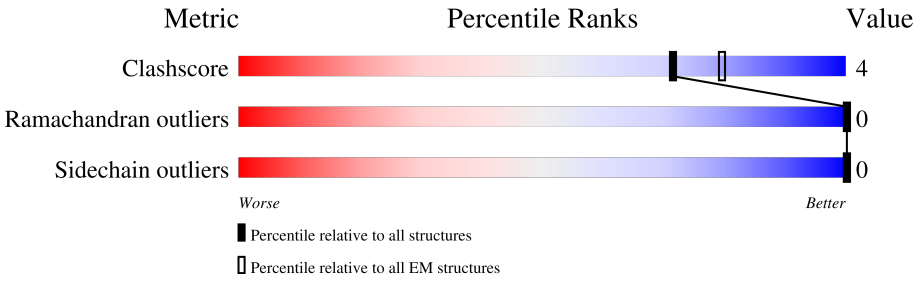
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 2.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	767	78% 6% 16%
2	B	278	77% 8% 15%
3	C	504	52% 7% 41%
4	D	529	46% 6% 48%
5	E	237	41% • 55%
6	F	250	46% • 52%
7	G	257	40% • 57%
8	H	257	44% 6% 50%

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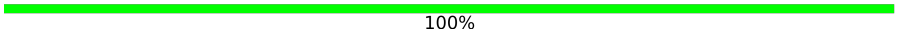
Mol	Chain	Length	Quality of chain
9	I	2	
9	J	2	
10	K	7	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 15656 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 Envelope glycoprotein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	647	5203	3331	881	967	24	0	0

There are 52 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	716	GLY	-	expression tag	UNP Q6SW67
A	717	THR	-	expression tag	UNP Q6SW67
A	718	LYS	-	expression tag	UNP Q6SW67
A	719	LEU	-	expression tag	UNP Q6SW67
A	720	GLY	-	expression tag	UNP Q6SW67
A	721	PRO	-	expression tag	UNP Q6SW67
A	722	GLU	-	expression tag	UNP Q6SW67
A	723	GLN	-	expression tag	UNP Q6SW67
A	724	LYS	-	expression tag	UNP Q6SW67
A	725	LEU	-	expression tag	UNP Q6SW67
A	726	ILE	-	expression tag	UNP Q6SW67
A	727	SER	-	expression tag	UNP Q6SW67
A	728	GLU	-	expression tag	UNP Q6SW67
A	729	GLU	-	expression tag	UNP Q6SW67
A	730	ASP	-	expression tag	UNP Q6SW67
A	731	LEU	-	expression tag	UNP Q6SW67
A	732	ASN	-	expression tag	UNP Q6SW67
A	733	SER	-	expression tag	UNP Q6SW67
A	734	ALA	-	expression tag	UNP Q6SW67
A	735	VAL	-	expression tag	UNP Q6SW67
A	736	ASP	-	expression tag	UNP Q6SW67
A	737	GLY	-	expression tag	UNP Q6SW67
A	738	SER	-	expression tag	UNP Q6SW67
A	739	GLY	-	expression tag	UNP Q6SW67
A	740	LEU	-	expression tag	UNP Q6SW67
A	741	ASN	-	expression tag	UNP Q6SW67
A	742	ASP	-	expression tag	UNP Q6SW67
A	743	ILE	-	expression tag	UNP Q6SW67

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Chain	Residue	Modelled	Actual	Comment	Reference
A	744	PHE	-	expression tag	UNP Q6SW67
A	745	GLU	-	expression tag	UNP Q6SW67
A	746	ALA	-	expression tag	UNP Q6SW67
A	747	GLN	-	expression tag	UNP Q6SW67
A	748	LYS	-	expression tag	UNP Q6SW67
A	749	ILE	-	expression tag	UNP Q6SW67
A	750	GLU	-	expression tag	UNP Q6SW67
A	751	TRP	-	expression tag	UNP Q6SW67
A	752	HIS	-	expression tag	UNP Q6SW67
A	753	GLU	-	expression tag	UNP Q6SW67
A	754	ASN	-	expression tag	UNP Q6SW67
A	755	LEU	-	expression tag	UNP Q6SW67
A	756	TYR	-	expression tag	UNP Q6SW67
A	757	PHE	-	expression tag	UNP Q6SW67
A	758	GLN	-	expression tag	UNP Q6SW67
A	759	GLY	-	expression tag	UNP Q6SW67
A	760	HIS	-	expression tag	UNP Q6SW67
A	761	HIS	-	expression tag	UNP Q6SW67
A	762	HIS	-	expression tag	UNP Q6SW67
A	763	HIS	-	expression tag	UNP Q6SW67
A	764	HIS	-	expression tag	UNP Q6SW67
A	765	HIS	-	expression tag	UNP Q6SW67
A	766	HIS	-	expression tag	UNP Q6SW67
A	767	HIS	-	expression tag	UNP Q6SW67

- Molecule 2 is a protein called Envelope glycoprotein L.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	236	Total	C	N	O	S	0	0
			1860	1183	325	344	8		

- Molecule 3 is a protein called Envelope glycoprotein O.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	299	Total	C	N	O	S	0	0
			2484	1602	426	440	16		

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	465	GLY	-	expression tag	UNP Q8BCU3
C	466	SER	-	expression tag	UNP Q8BCU3

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Chain	Residue	Modelled	Actual	Comment	Reference
C	467	GLU	-	expression tag	UNP Q8BCU3
C	468	ASN	-	expression tag	UNP Q8BCU3
C	469	LEU	-	expression tag	UNP Q8BCU3
C	470	TYR	-	expression tag	UNP Q8BCU3
C	471	PHE	-	expression tag	UNP Q8BCU3
C	472	GLN	-	expression tag	UNP Q8BCU3
C	473	GLY	-	expression tag	UNP Q8BCU3
C	474	SER	-	expression tag	UNP Q8BCU3
C	475	ALA	-	expression tag	UNP Q8BCU3
C	476	TRP	-	expression tag	UNP Q8BCU3
C	477	SER	-	expression tag	UNP Q8BCU3
C	478	HIS	-	expression tag	UNP Q8BCU3
C	479	PRO	-	expression tag	UNP Q8BCU3
C	480	GLN	-	expression tag	UNP Q8BCU3
C	481	PHE	-	expression tag	UNP Q8BCU3
C	482	GLU	-	expression tag	UNP Q8BCU3
C	483	LYS	-	expression tag	UNP Q8BCU3
C	484	GLY	-	expression tag	UNP Q8BCU3
C	485	GLY	-	expression tag	UNP Q8BCU3
C	486	GLY	-	expression tag	UNP Q8BCU3
C	487	SER	-	expression tag	UNP Q8BCU3
C	488	GLY	-	expression tag	UNP Q8BCU3
C	489	GLY	-	expression tag	UNP Q8BCU3
C	490	GLY	-	expression tag	UNP Q8BCU3
C	491	SER	-	expression tag	UNP Q8BCU3
C	492	GLY	-	expression tag	UNP Q8BCU3
C	493	GLY	-	expression tag	UNP Q8BCU3
C	494	GLY	-	expression tag	UNP Q8BCU3
C	495	SER	-	expression tag	UNP Q8BCU3
C	496	ALA	-	expression tag	UNP Q8BCU3
C	497	TRP	-	expression tag	UNP Q8BCU3
C	498	SER	-	expression tag	UNP Q8BCU3
C	499	HIS	-	expression tag	UNP Q8BCU3
C	500	PRO	-	expression tag	UNP Q8BCU3
C	501	GLN	-	expression tag	UNP Q8BCU3
C	502	PHE	-	expression tag	UNP Q8BCU3
C	503	GLU	-	expression tag	UNP Q8BCU3
C	504	LYS	-	expression tag	UNP Q8BCU3

- Molecule 4 is a protein called Isoform 3 of Platelet-derived growth factor receptor alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	274	Total	C	N	O	S	0	0
			2142	1359	339	433	11		

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	525	ASP	-	expression tag	UNP P16234
D	526	ASP	-	expression tag	UNP P16234
D	527	ASP	-	expression tag	UNP P16234
D	528	ASP	-	expression tag	UNP P16234
D	529	LYS	-	expression tag	UNP P16234

- Molecule 5 is a protein called Fab 13H11 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	106	Total	C	N	O	S	0	0
			798	506	132	157	3		

- Molecule 6 is a protein called Fab 13H11 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	121	Total	C	N	O	S	0	0
			927	583	161	178	5		

- Molecule 7 is a protein called Fab MSL-109 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	111	Total	C	N	O	S	0	0
			850	534	143	169	4		

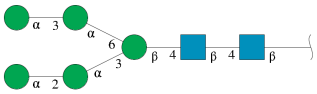
- Molecule 8 is a protein called Fab MSL-109 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	129	Total	C	N	O	S	0	0
			1001	635	165	198	3		

- Molecule 9 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

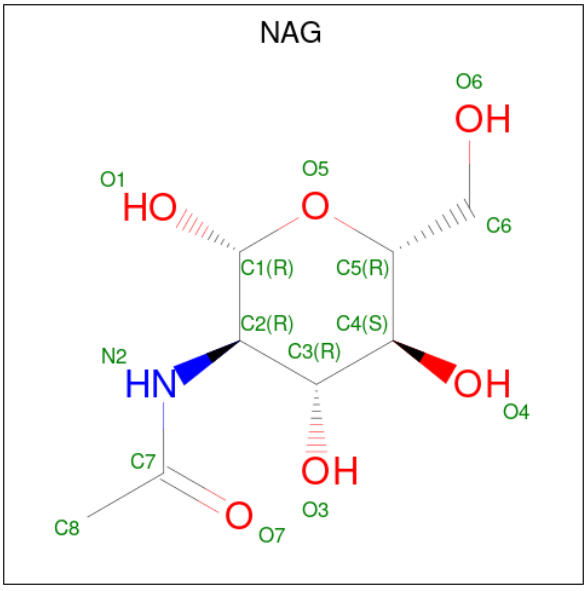
Mol	Chain	Residues	Atoms	AltConf	Trace
9	I	2	Total C N O 28 16 2 10	0	0
9	J	2	Total C N O 28 16 2 10	0	0

- Molecule 10 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-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
10	K	7	Total C N O 83 46 2 35	0	0

- Molecule 11 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms	AltConf
11	A	1	Total C N O 70 40 5 25	0
11	A	1	Total C N O 70 40 5 25	0

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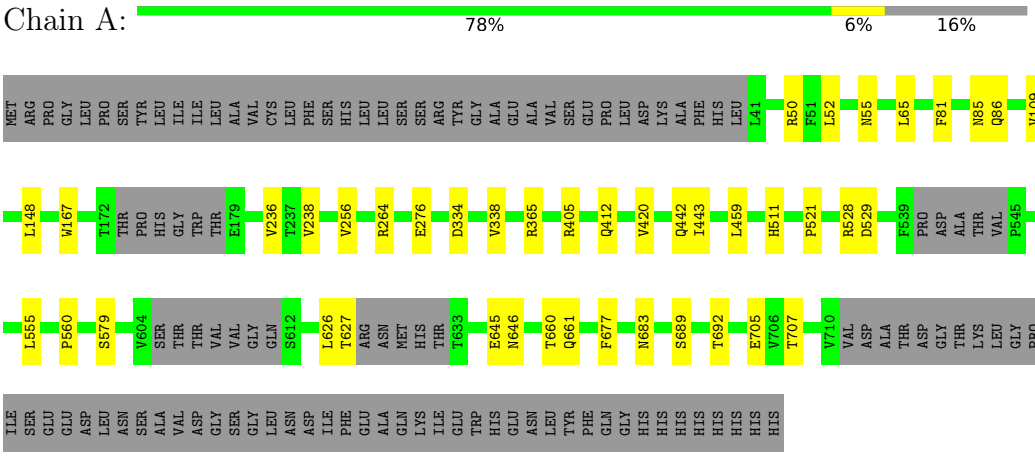
Mol	Chain	Residues	Atoms	AltConf
11	A	1	Total C N O 70 40 5 25	0
11	A	1	Total C N O 70 40 5 25	0
11	A	1	Total C N O 70 40 5 25	0
11	B	1	Total C N O 14 8 1 5	0
11	C	1	Total C N O 140 80 10 50	0
11	C	1	Total C N O 140 80 10 50	0
11	C	1	Total C N O 140 80 10 50	0
11	C	1	Total C N O 140 80 10 50	0
11	C	1	Total C N O 140 80 10 50	0
11	C	1	Total C N O 140 80 10 50	0
11	C	1	Total C N O 140 80 10 50	0
11	C	1	Total C N O 140 80 10 50	0
11	C	1	Total C N O 140 80 10 50	0
11	C	1	Total C N O 140 80 10 50	0
11	D	1	Total C N O 28 16 2 10	0
11	D	1	Total C N O 28 16 2 10	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 = 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.

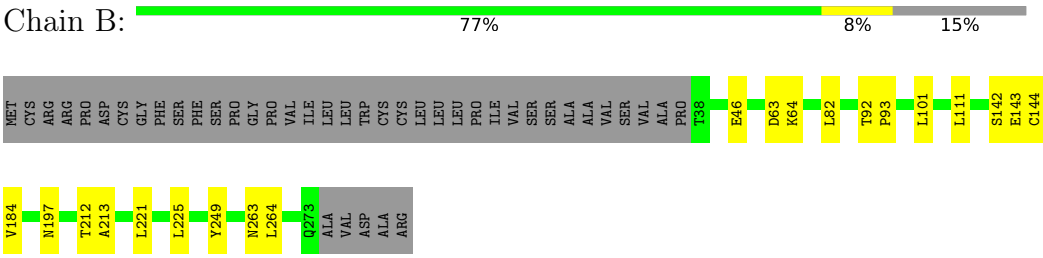
• Molecule 1: Envelope glycoprotein H

Chain A:



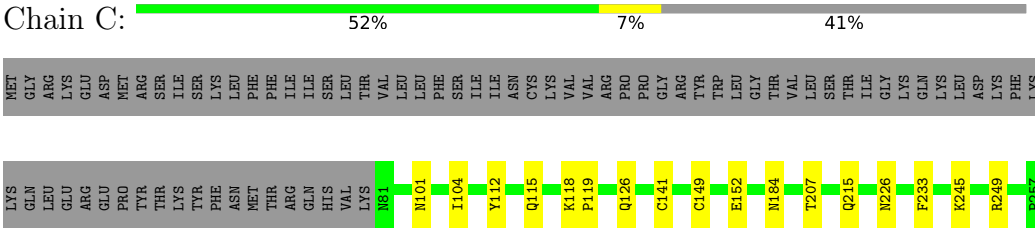
• Molecule 2: Envelope glycoprotein L

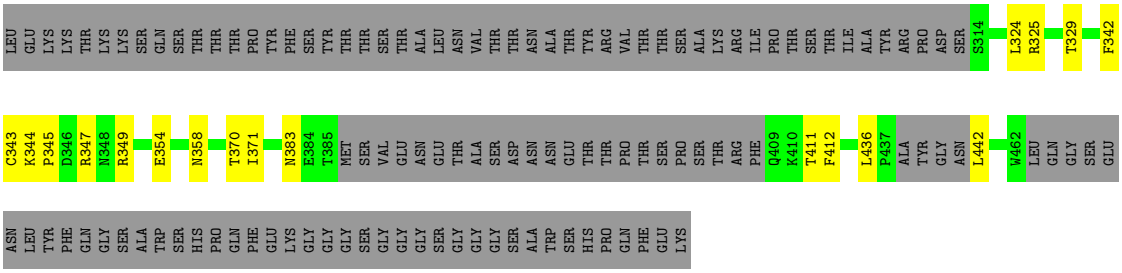
Chain B:



• Molecule 3: Envelope glycoprotein O

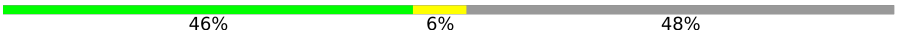
Chain C:

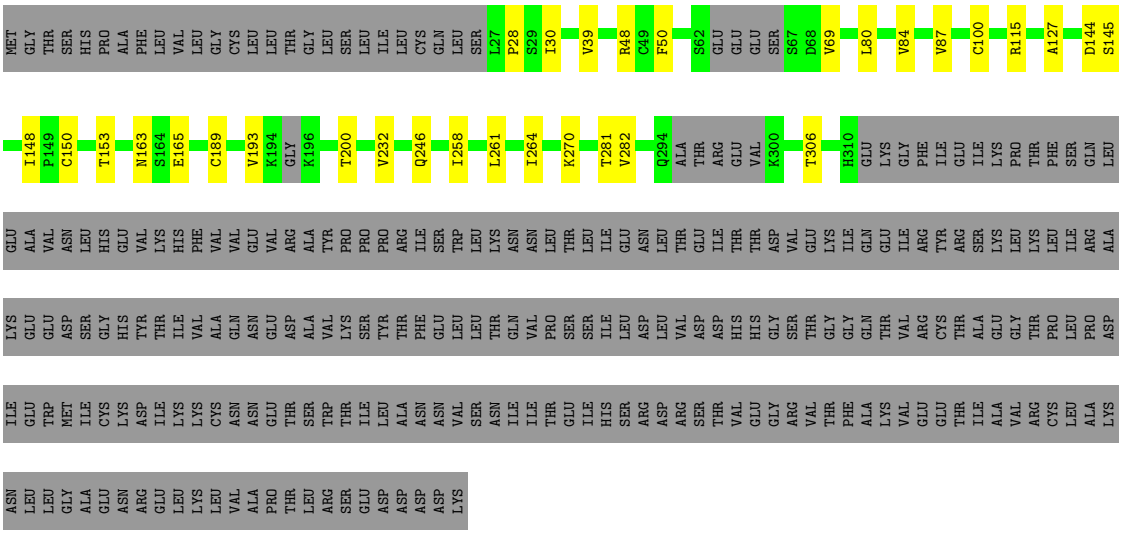




• Molecule 4: Isoform 3 of Platelet-derived growth factor receptor alpha

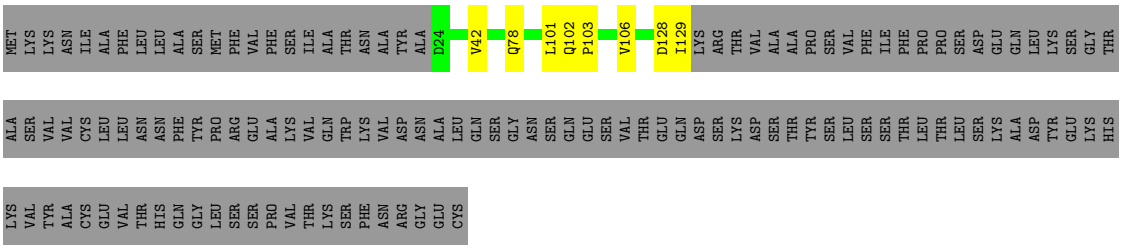
Chain D:





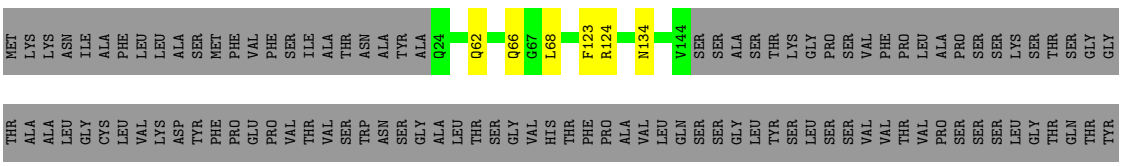
• Molecule 5: Fab 13H11 light chain

Chain E:



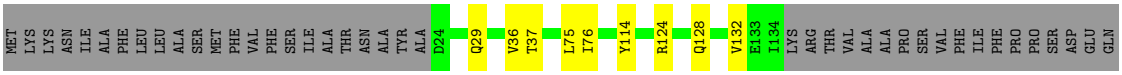
• Molecule 6: Fab 13H11 heavy chain

Chain F:



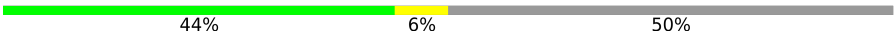
• Molecule 7: Fab MSL-109 light chain

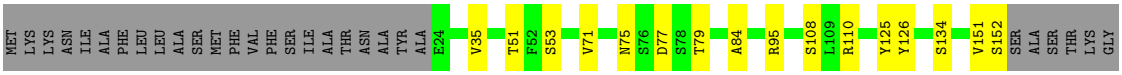
Chain G:

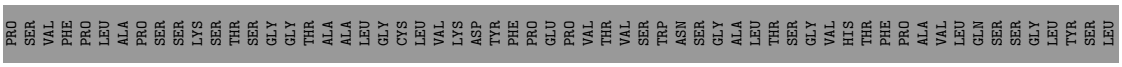


• Molecule 8: Fab MSL-109 heavy chain

Chain H:





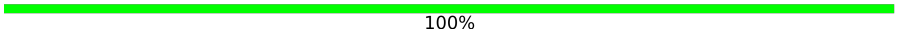


• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

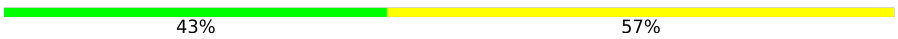
• Molecule 9: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

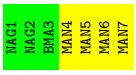
Chain J:



• Molecule 10: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-3)-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:





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	3560620	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	165000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	52.082	Depositor
Minimum map value	-21.646	Depositor
Average map value	-0.033	Depositor
Map value standard deviation	0.674	Depositor
Recommended contour level	3.2	Depositor
Map size (Å)	356.7696, 356.7696, 356.7696	wwPDB
Map dimensions	264, 264, 264	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3514, 1.3514, 1.3514	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, MAN, BMA

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	0.24	0/5322	0.48	0/7245
2	B	0.26	0/1905	0.51	0/2601
3	C	0.26	0/2552	0.51	0/3465
4	D	0.26	0/2185	0.47	0/2975
5	E	0.26	0/816	0.50	0/1111
6	F	0.26	0/947	0.52	0/1284
7	G	0.27	0/868	0.49	0/1180
8	H	0.27	0/1026	0.50	0/1391
All	All	0.26	0/15621	0.49	0/21252

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	5203	0	5162	32	0
2	B	1860	0	1851	16	0
3	C	2484	0	2455	24	0
4	D	2142	0	2078	21	0
5	E	798	0	788	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	F	927	0	903	6	0
7	G	850	0	831	5	0
8	H	1001	0	938	10	0
9	I	28	0	25	1	0
9	J	28	0	25	0	0
10	K	83	0	70	0	0
11	A	70	0	65	1	0
11	B	14	0	13	0	0
11	C	140	0	130	2	0
11	D	28	0	26	0	0
All	All	15656	0	15360	109	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 4.

All (109) 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)
6:F:62:GLN:NE2	6:F:66:GLN:O	2.10	0.84
1:A:264:ARG:NH1	1:A:276:GLU:OE1	2.14	0.81
1:A:705:GLU:OE2	1:A:707:THR:HG22	1.84	0.75
7:G:29:GLN:O	7:G:128:GLN:NE2	2.23	0.72
3:C:345:PRO:O	3:C:349:ARG:NH2	2.23	0.72
1:A:65:LEU:HD21	1:A:86:GLN:OE1	1.92	0.69
1:A:113:GLU:HG3	1:A:117:ARG:HD3	1.78	0.66
2:B:111:LEU:O	2:B:197:ASN:ND2	2.31	0.64
3:C:354:GLU:O	3:C:358:ASN:ND2	2.31	0.64
5:E:78:GLN:NE2	6:F:134:ASN:OD1	2.31	0.63
6:F:62:GLN:OE1	6:F:68:LEU:HD23	1.98	0.62
1:A:167:TRP:O	1:A:442:GLN:NE2	2.33	0.62
1:A:677:PHE:O	1:A:683:ASN:ND2	2.33	0.61
3:C:383:ASN:HD21	11:C:607:NAG:C1	2.13	0.61
4:D:30:ILE:HD11	4:D:100:CYS:HB3	1.82	0.60
1:A:256:VAL:O	1:A:264:ARG:NH2	2.32	0.60
3:C:344:LYS:NZ	4:D:246:GLN:OE1	2.35	0.60
3:C:207:THR:HG23	3:C:324:LEU:CD2	2.32	0.60
3:C:207:THR:HG23	3:C:324:LEU:HD21	1.85	0.59
8:H:51:THR:HG22	8:H:53:SER:H	1.66	0.59
1:A:55:ASN:HD21	11:A:803:NAG:C1	2.16	0.58
7:G:75:LEU:HB3	7:G:76:ILE:HD12	1.85	0.57
3:C:101:ASN:HD21	11:C:602:NAG:C1	2.17	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:42:VAL:HG21	5:E:101:LEU:HD12	1.86	0.57
3:C:436:LEU:O	3:C:436:LEU:HD23	2.05	0.56
1:A:548:VAL:HG23	1:A:549:PRO:HD3	1.87	0.56
1:A:528:ARG:NH2	1:A:560:PRO:O	2.39	0.56
4:D:163:ASN:ND2	4:D:165:GLU:OE1	2.39	0.56
1:A:626:LEU:O	1:A:627:THR:OG1	2.22	0.55
1:A:81:PHE:CB	2:B:184:VAL:HG12	2.36	0.55
4:D:264:ILE:HD11	4:D:270:LYS:HE2	1.89	0.55
2:B:183:LEU:HD23	2:B:249:TYR:CD2	2.42	0.55
8:H:35:VAL:O	8:H:152:SER:N	2.37	0.54
3:C:141:CYS:HB2	3:C:149:CYS:HA	1.89	0.53
1:A:511:HIS:ND1	1:A:511:HIS:O	2.41	0.52
1:A:405:ARG:NE	1:A:412:GLN:OE1	2.35	0.52
2:B:142:SER:N	3:C:184:ASN:OD1	2.36	0.52
5:E:128:ASP:OD1	5:E:129:ILE:N	2.42	0.52
3:C:325:ARG:O	3:C:329:THR:HG23	2.10	0.52
2:B:92:THR:N	2:B:93:PRO:HD2	2.25	0.51
1:A:420:VAL:HG22	1:A:443:ILE:HG12	1.92	0.51
6:F:123:PHE:CZ	6:F:124:ARG:NH1	2.79	0.51
4:D:50:PHE:HB3	4:D:80:LEU:HD21	1.92	0.51
1:A:81:PHE:HB3	2:B:184:VAL:HG12	1.93	0.50
3:C:245:LYS:HG2	3:C:249:ARG:NH1	2.26	0.50
4:D:258:ILE:HD11	9:I:1:NAG:H83	1.92	0.50
8:H:75:ASN:ND2	8:H:77:ASP:OD1	2.44	0.50
4:D:28:PRO:O	4:D:115:ARG:NE	2.39	0.49
5:E:102:GLN:NE2	5:E:103:PRO:HD2	2.27	0.49
8:H:71:VAL:O	8:H:84:ALA:N	2.44	0.49
1:A:689:SER:O	1:A:692:THR:OG1	2.30	0.48
2:B:46:GLU:OE1	2:B:46:GLU:N	2.41	0.48
3:C:411:THR:HG22	3:C:412:PHE:N	2.29	0.48
4:D:39:VAL:O	4:D:39:VAL:HG13	2.13	0.48
4:D:127:ALA:O	4:D:153:THR:HG22	2.14	0.48
6:F:123:PHE:CE2	6:F:124:ARG:NH1	2.82	0.47
5:E:106:VAL:O	5:E:106:VAL:HG23	2.15	0.47
8:H:75:ASN:O	8:H:95:ARG:NH1	2.46	0.47
1:A:334:ASP:O	1:A:338:VAL:HG23	2.16	0.46
4:D:127:ALA:HB2	4:D:193:VAL:HG21	1.96	0.46
2:B:221:LEU:O	2:B:225:LEU:HD23	2.14	0.46
4:D:144:ASP:OD1	4:D:145:SER:N	2.49	0.46
3:C:342:PHE:CE1	4:D:261:LEU:HD22	2.51	0.46
3:C:370:THR:HG22	3:C:371:ILE:N	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:551:ALA:O	1:A:555:LEU:HD13	2.15	0.46
2:B:82:LEU:O	2:B:170:GLY:N	2.43	0.46
1:A:645:GLU:O	1:A:646:ASN:OD1	2.34	0.45
2:B:63:ASP:OD1	2:B:64:LYS:N	2.49	0.45
2:B:212:THR:HG22	2:B:213:ALA:N	2.32	0.45
3:C:118:LYS:HB2	3:C:119:PRO:HA	1.99	0.45
4:D:48:ARG:HA	4:D:84:VAL:HA	1.97	0.45
4:D:189:CYS:SG	4:D:200:THR:OG1	2.65	0.45
4:D:69:VAL:HG12	4:D:87:VAL:HG12	1.98	0.45
4:D:281:THR:HG22	4:D:282:VAL:N	2.31	0.45
8:H:108:SER:O	8:H:110:ARG:NH1	2.50	0.45
1:A:238:VAL:HG13	1:A:238:VAL:O	2.17	0.45
3:C:141:CYS:HB3	3:C:152:GLU:OE1	2.17	0.45
2:B:144:CYS:SG	3:C:347:ARG:NH1	2.90	0.44
8:H:110:ARG:O	8:H:151:VAL:HG11	2.17	0.44
3:C:436:LEU:HD11	3:C:442:LEU:HA	1.99	0.44
2:B:101:LEU:HD13	3:C:233:PHE:HB3	1.99	0.44
7:G:114:TYR:CE1	7:G:132:VAL:HG21	2.52	0.44
8:H:77:ASP:OD1	8:H:79:THR:OG1	2.36	0.44
7:G:36:VAL:HG12	7:G:37:THR:N	2.33	0.44
1:A:459:LEU:HD22	1:A:521:PRO:HD3	2.00	0.44
2:B:263:ASN:C	2:B:264:LEU:HD22	2.39	0.43
3:C:343:CYS:HA	3:C:347:ARG:HD2	2.00	0.43
1:A:660:THR:HG23	1:A:661:GLN:N	2.33	0.43
2:B:143:GLU:HG3	2:B:144:CYS:N	2.33	0.43
1:A:85:ASN:OD1	1:A:85:ASN:C	2.57	0.43
8:H:125:TYR:O	8:H:134:SER:OG	2.26	0.42
1:A:109:VAL:HG13	1:A:109:VAL:O	2.19	0.42
4:D:30:ILE:HD13	4:D:115:ARG:HG3	2.02	0.42
7:G:124:ARG:NH2	8:H:126:TYR:OH	2.52	0.42
1:A:548:VAL:CG2	1:A:549:PRO:HD3	2.48	0.42
4:D:232:VAL:O	4:D:232:VAL:HG23	2.20	0.42
4:D:30:ILE:HD11	4:D:100:CYS:CB	2.50	0.41
6:F:123:PHE:CE2	6:F:124:ARG:CZ	3.03	0.41
3:C:104:ILE:HD11	3:C:126:GLN:HG3	2.01	0.41
1:A:529:ASP:OD2	1:A:579:SER:OG	2.37	0.41
4:D:306:THR:O	4:D:306:THR:HG23	2.20	0.41
1:A:81:PHE:HB2	2:B:184:VAL:HG12	2.00	0.41
1:A:148:LEU:O	1:A:365:ARG:HD3	2.21	0.41
1:A:645:GLU:OE1	1:A:646:ASN:ND2	2.54	0.41
3:C:215:GLN:OE1	3:C:226:ASN:ND2	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:VAL:O	1:A:236:VAL:HG13	2.20	0.41
4:D:148:ILE:O	4:D:150:CYS:N	2.51	0.40
3:C:112:TYR:O	3:C:115:GLN:O	2.40	0.40
1:A:50:ARG:NH1	1:A:52:LEU:HD21	2.36	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	637/767 (83%)	619 (97%)	18 (3%)	0	100	100
2	B	234/278 (84%)	228 (97%)	6 (3%)	0	100	100
3	C	291/504 (58%)	284 (98%)	7 (2%)	0	100	100
4	D	266/529 (50%)	259 (97%)	7 (3%)	0	100	100
5	E	104/237 (44%)	102 (98%)	2 (2%)	0	100	100
6	F	119/250 (48%)	118 (99%)	1 (1%)	0	100	100
7	G	109/257 (42%)	106 (97%)	3 (3%)	0	100	100
8	H	127/257 (49%)	125 (98%)	2 (2%)	0	100	100
All	All	1887/3079 (61%)	1841 (98%)	46 (2%)	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	589/692 (85%)	589 (100%)	0	100	100
2	B	203/238 (85%)	203 (100%)	0	100	100
3	C	279/460 (61%)	279 (100%)	0	100	100
4	D	246/475 (52%)	246 (100%)	0	100	100
5	E	89/204 (44%)	89 (100%)	0	100	100
6	F	101/211 (48%)	101 (100%)	0	100	100
7	G	97/225 (43%)	97 (100%)	0	100	100
8	H	106/216 (49%)	106 (100%)	0	100	100
All	All	1710/2721 (63%)	1710 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

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

Mol	Chain	Res	Type
3	C	101	ASN
3	C	383	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)

11 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	$\#\|Z\|>2$
9	NAG	I	1	3,9	14,14,15	0.21	0	17,19,21	0.48	0
9	NAG	I	2	9	14,14,15	0.21	0	17,19,21	0.43	0
9	NAG	J	1	3,9	14,14,15	0.26	0	17,19,21	0.44	0
9	NAG	J	2	9	14,14,15	0.22	0	17,19,21	0.43	0
10	NAG	K	1	3,10	14,14,15	0.25	0	17,19,21	0.47	0
10	NAG	K	2	10	14,14,15	0.23	0	17,19,21	0.42	0
10	BMA	K	3	10	11,11,12	0.60	0	15,15,17	0.98	0
10	MAN	K	4	10	11,11,12	0.57	0	15,15,17	1.05	2 (13%)
10	MAN	K	5	10	11,11,12	0.62	0	15,15,17	0.89	1 (6%)
10	MAN	K	6	10	11,11,12	0.65	0	15,15,17	1.04	2 (13%)
10	MAN	K	7	10	11,11,12	0.61	0	15,15,17	0.95	2 (13%)

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
9	NAG	I	1	3,9	-	2/6/23/26	0/1/1/1
9	NAG	I	2	9	-	0/6/23/26	0/1/1/1
9	NAG	J	1	3,9	-	0/6/23/26	0/1/1/1
9	NAG	J	2	9	-	1/6/23/26	0/1/1/1
10	NAG	K	1	3,10	-	0/6/23/26	0/1/1/1
10	NAG	K	2	10	-	0/6/23/26	0/1/1/1
10	BMA	K	3	10	-	0/2/19/22	0/1/1/1
10	MAN	K	4	10	-	0/2/19/22	0/1/1/1
10	MAN	K	5	10	-	2/2/19/22	0/1/1/1
10	MAN	K	6	10	-	0/2/19/22	0/1/1/1
10	MAN	K	7	10	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	K	4	MAN	O2-C2-C3	-2.67	104.78	110.14
10	K	6	MAN	O2-C2-C3	-2.46	105.22	110.14
10	K	4	MAN	C1-O5-C5	2.29	115.30	112.19
10	K	7	MAN	O2-C2-C3	-2.25	105.62	110.14
10	K	6	MAN	C1-O5-C5	2.18	115.14	112.19
10	K	7	MAN	C1-O5-C5	2.16	115.11	112.19
10	K	5	MAN	O2-C2-C3	-2.15	105.83	110.14

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	J	2	NAG	O5-C5-C6-O6
10	K	5	MAN	O5-C5-C6-O6
10	K	5	MAN	C4-C5-C6-O6
9	I	1	NAG	C1-C2-N2-C7
9	I	1	NAG	C3-C2-N2-C7

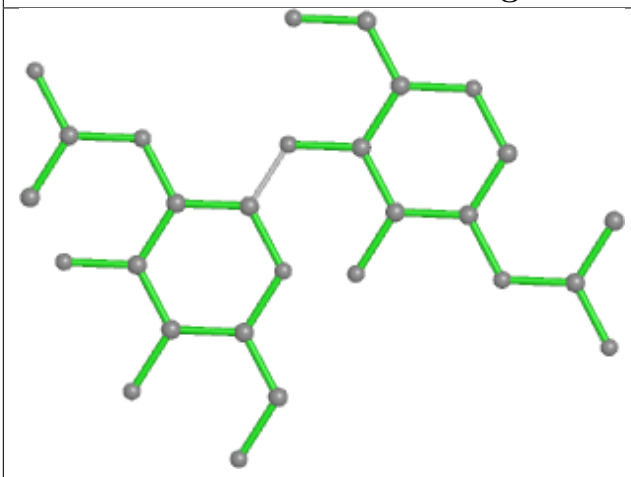
There are no ring outliers.

1 monomer is involved in 1 short contact:

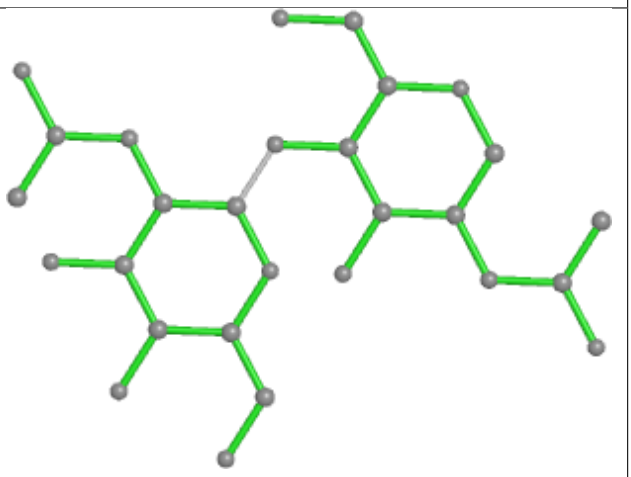
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	1	NAG	1	0

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

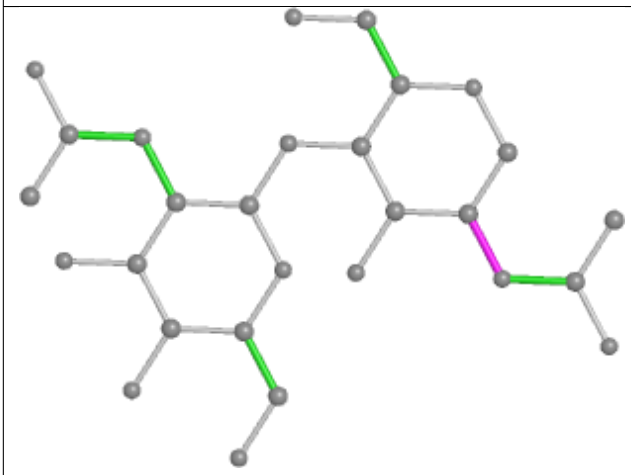
Oligosaccharide Chain I



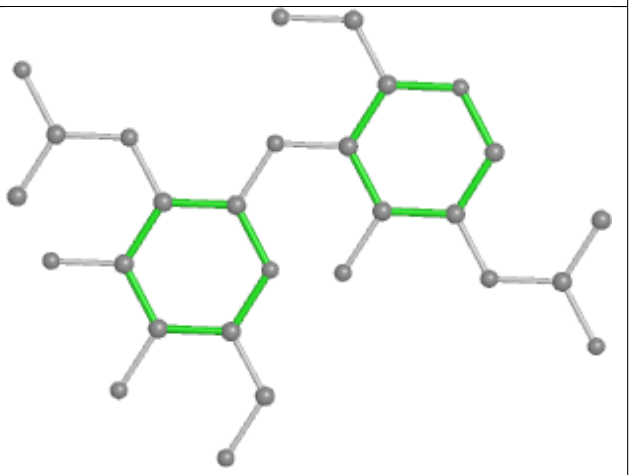
Bond lengths



Bond angles

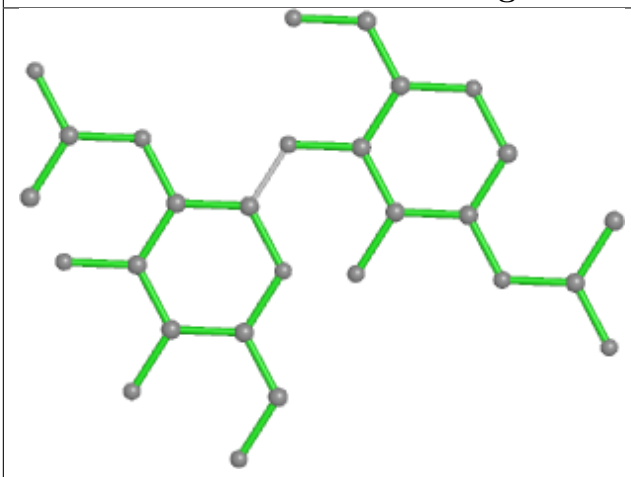


Torsions

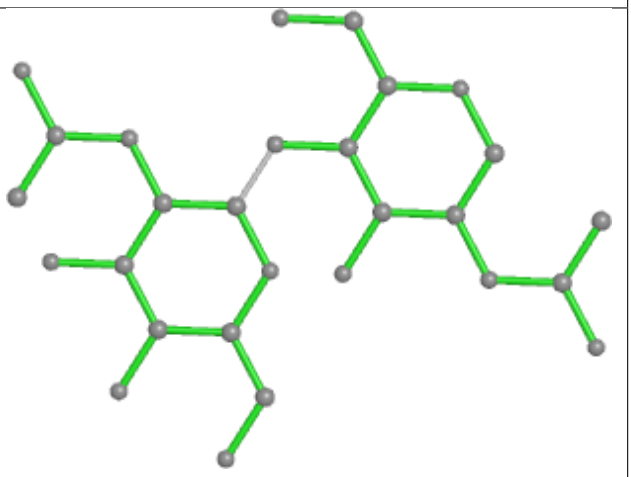


Rings

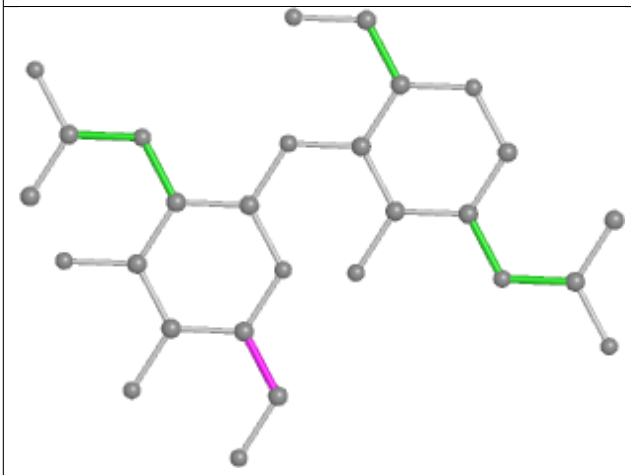
Oligosaccharide Chain J



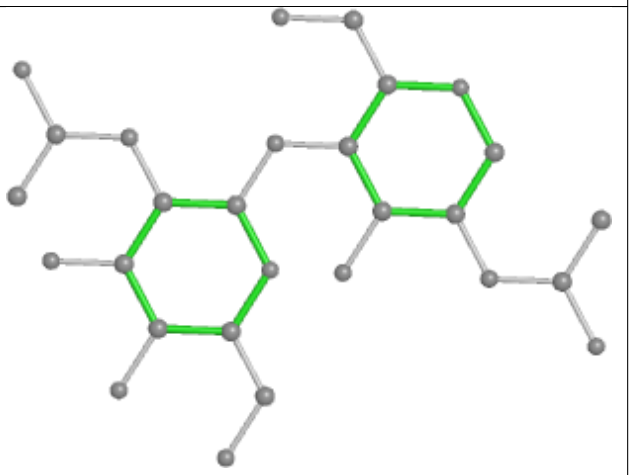
Bond lengths



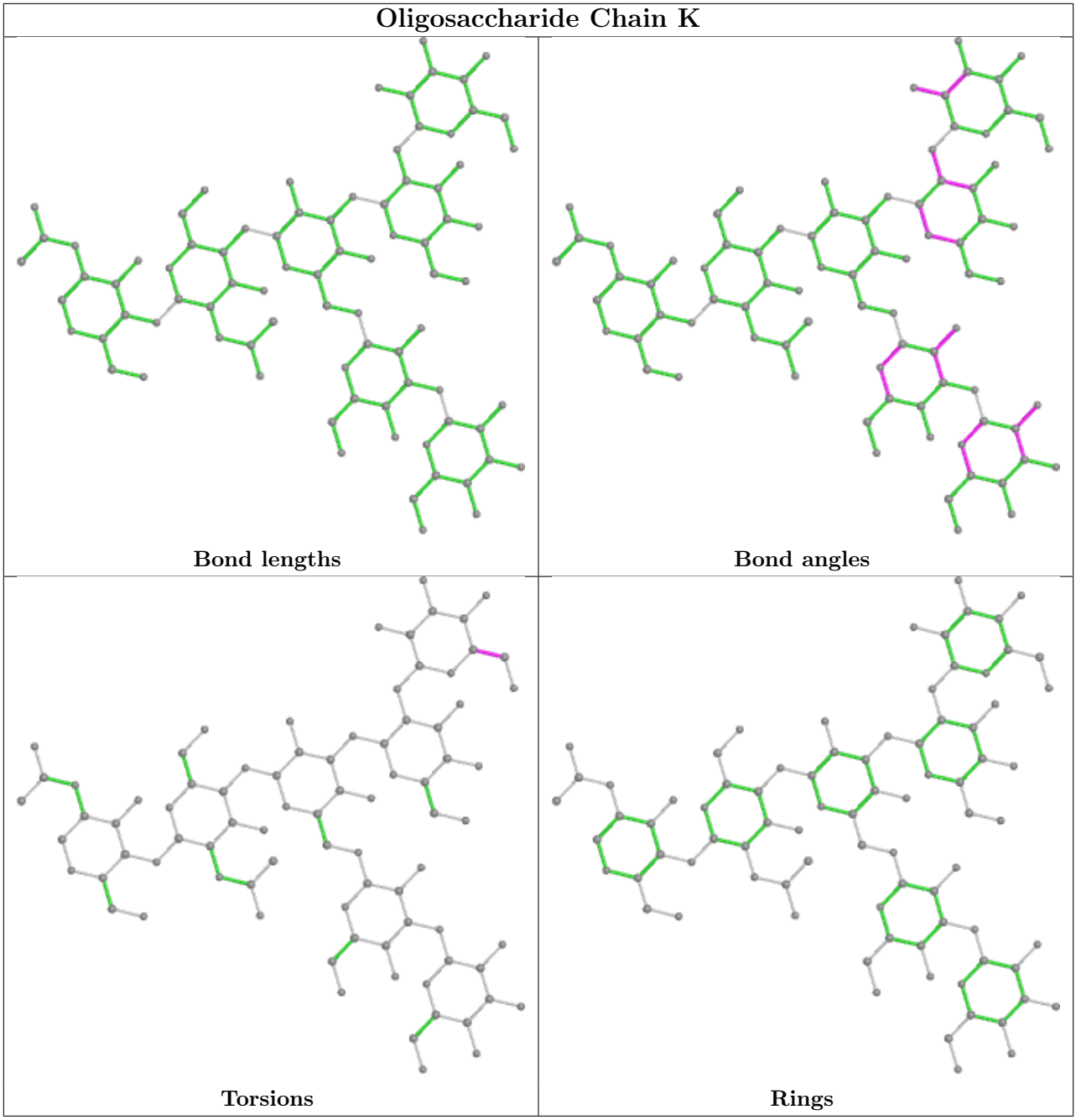
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

18 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	$\#\|Z\|>2$
11	NAG	A	802	-	14,14,15	0.22	0	17,19,21	0.41	0
11	NAG	A	805	-	14,14,15	0.22	0	17,19,21	0.41	0
11	NAG	B	301	2	14,14,15	0.21	0	17,19,21	0.39	0
11	NAG	C	603	3	14,14,15	0.20	0	17,19,21	0.44	0
11	NAG	C	605	3	14,14,15	0.22	0	17,19,21	0.42	0
11	NAG	C	606	3	14,14,15	0.21	0	17,19,21	0.37	0
11	NAG	C	609	-	14,14,15	0.24	0	17,19,21	0.40	0
11	NAG	C	604	3	14,14,15	0.20	0	17,19,21	0.45	0
11	NAG	D	601	4	14,14,15	0.19	0	17,19,21	0.45	0
11	NAG	C	610	-	14,14,15	0.21	0	17,19,21	0.40	0
11	NAG	C	607	-	14,14,15	0.22	0	17,19,21	0.41	0
11	NAG	A	803	-	14,14,15	0.21	0	17,19,21	0.41	0
11	NAG	A	801	1	14,14,15	0.19	0	17,19,21	0.41	0
11	NAG	C	601	3	14,14,15	0.22	0	17,19,21	0.35	0
11	NAG	A	804	1	14,14,15	0.20	0	17,19,21	0.45	0
11	NAG	C	608	3	14,14,15	0.21	0	17,19,21	0.46	0
11	NAG	C	602	-	14,14,15	0.19	0	17,19,21	0.42	0
11	NAG	D	602	4	14,14,15	0.24	0	17,19,21	0.47	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
11	NAG	A	802	-	-	3/6/23/26	0/1/1/1
11	NAG	A	805	-	-	0/6/23/26	0/1/1/1
11	NAG	B	301	2	-	0/6/23/26	0/1/1/1
11	NAG	C	603	3	-	0/6/23/26	0/1/1/1
11	NAG	C	605	3	-	0/6/23/26	0/1/1/1
11	NAG	C	606	3	-	2/6/23/26	0/1/1/1
11	NAG	C	609	-	-	1/6/23/26	0/1/1/1
11	NAG	C	604	3	-	2/6/23/26	0/1/1/1
11	NAG	D	601	4	-	1/6/23/26	0/1/1/1
11	NAG	C	610	-	-	0/6/23/26	0/1/1/1
11	NAG	C	607	-	-	2/6/23/26	0/1/1/1
11	NAG	A	803	-	-	3/6/23/26	0/1/1/1
11	NAG	A	801	1	-	0/6/23/26	0/1/1/1
11	NAG	C	601	3	-	2/6/23/26	0/1/1/1
11	NAG	A	804	1	-	0/6/23/26	0/1/1/1
11	NAG	C	608	3	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	NAG	C	602	-	-	2/6/23/26	0/1/1/1
11	NAG	D	602	4	-	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 (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	607	NAG	O5-C5-C6-O6
11	A	802	NAG	O5-C5-C6-O6
11	C	602	NAG	O5-C5-C6-O6
11	C	607	NAG	C4-C5-C6-O6
11	C	609	NAG	O5-C5-C6-O6
11	A	803	NAG	O5-C5-C6-O6
11	C	606	NAG	O5-C5-C6-O6
11	C	602	NAG	C4-C5-C6-O6
11	C	601	NAG	O5-C5-C6-O6
11	D	601	NAG	O5-C5-C6-O6
11	A	802	NAG	C4-C5-C6-O6
11	C	608	NAG	C4-C5-C6-O6
11	C	608	NAG	O5-C5-C6-O6
11	D	602	NAG	C4-C5-C6-O6
11	D	602	NAG	O5-C5-C6-O6
11	C	601	NAG	C1-C2-N2-C7
11	A	803	NAG	C3-C2-N2-C7
11	C	604	NAG	C3-C2-N2-C7
11	C	606	NAG	C3-C2-N2-C7
11	C	608	NAG	C3-C2-N2-C7
11	A	803	NAG	C1-C2-N2-C7
11	C	604	NAG	O5-C5-C6-O6
11	A	802	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	C	607	NAG	1	0
11	A	803	NAG	1	0
11	C	602	NAG	1	0

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.

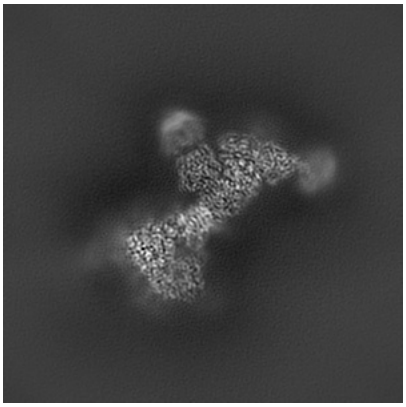
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-23253. These allow visual inspection of the internal detail of the map and identification of artifacts.

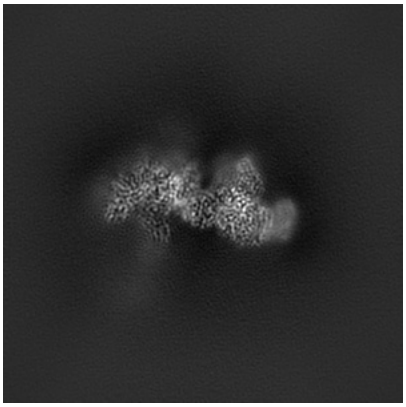
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

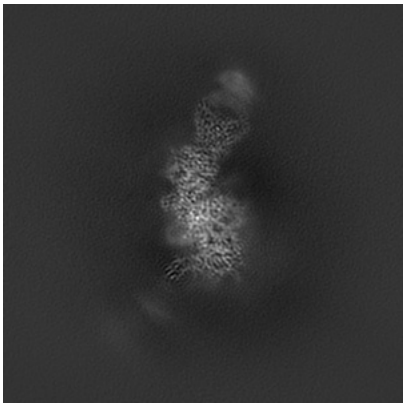
6.1.1 Primary map



X



Y

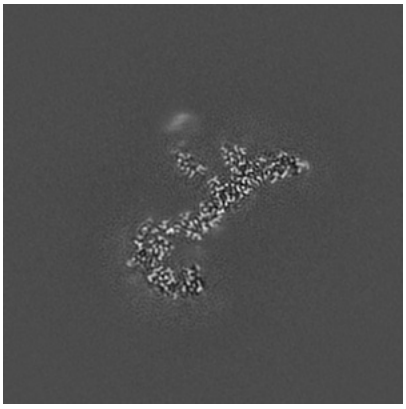


Z

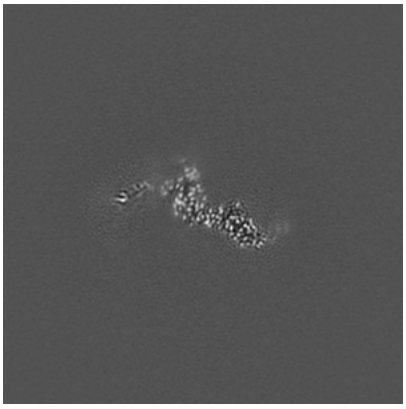
The images above show the map projected in three orthogonal directions.

6.2 Central slices

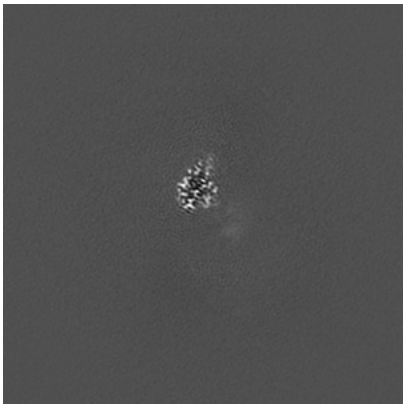
6.2.1 Primary map



X Index: 132



Y Index: 132

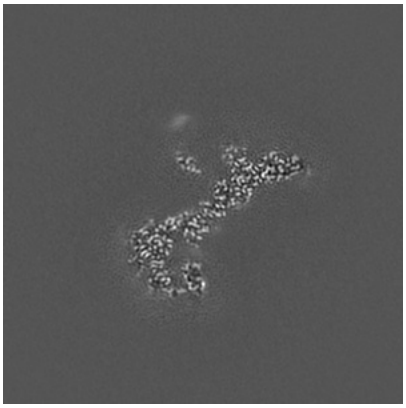


Z Index: 132

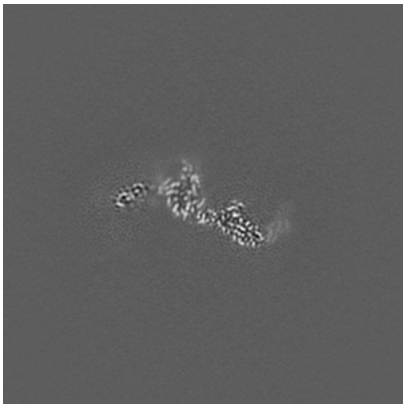
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

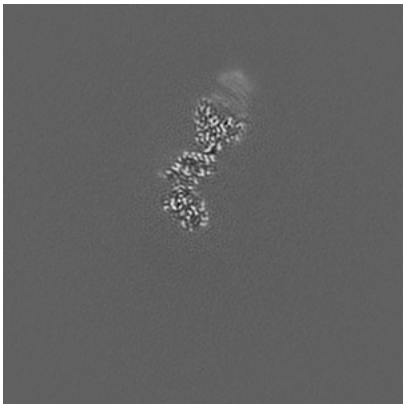
6.3.1 Primary map



X Index: 134



Y Index: 130

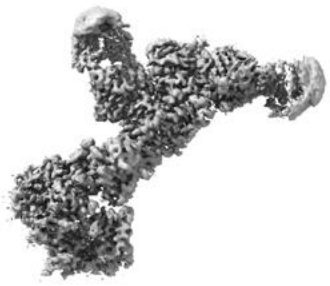


Z Index: 155

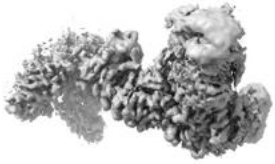
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map



X



Y

Z

The images above show the 3D surface view of the map at the recommended contour level 3.2. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

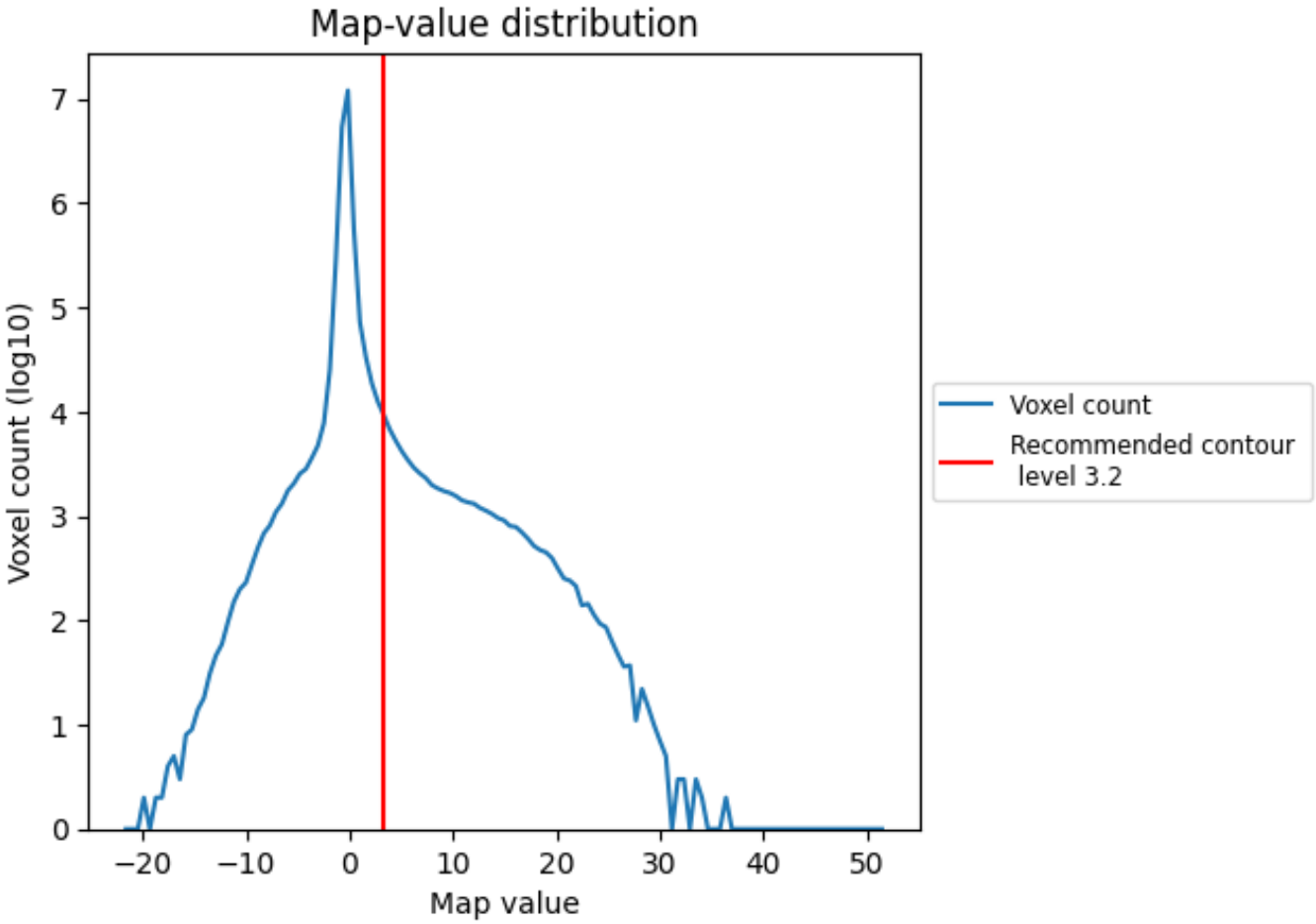
6.5 Mask visualisation (i)

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

7 Map analysis

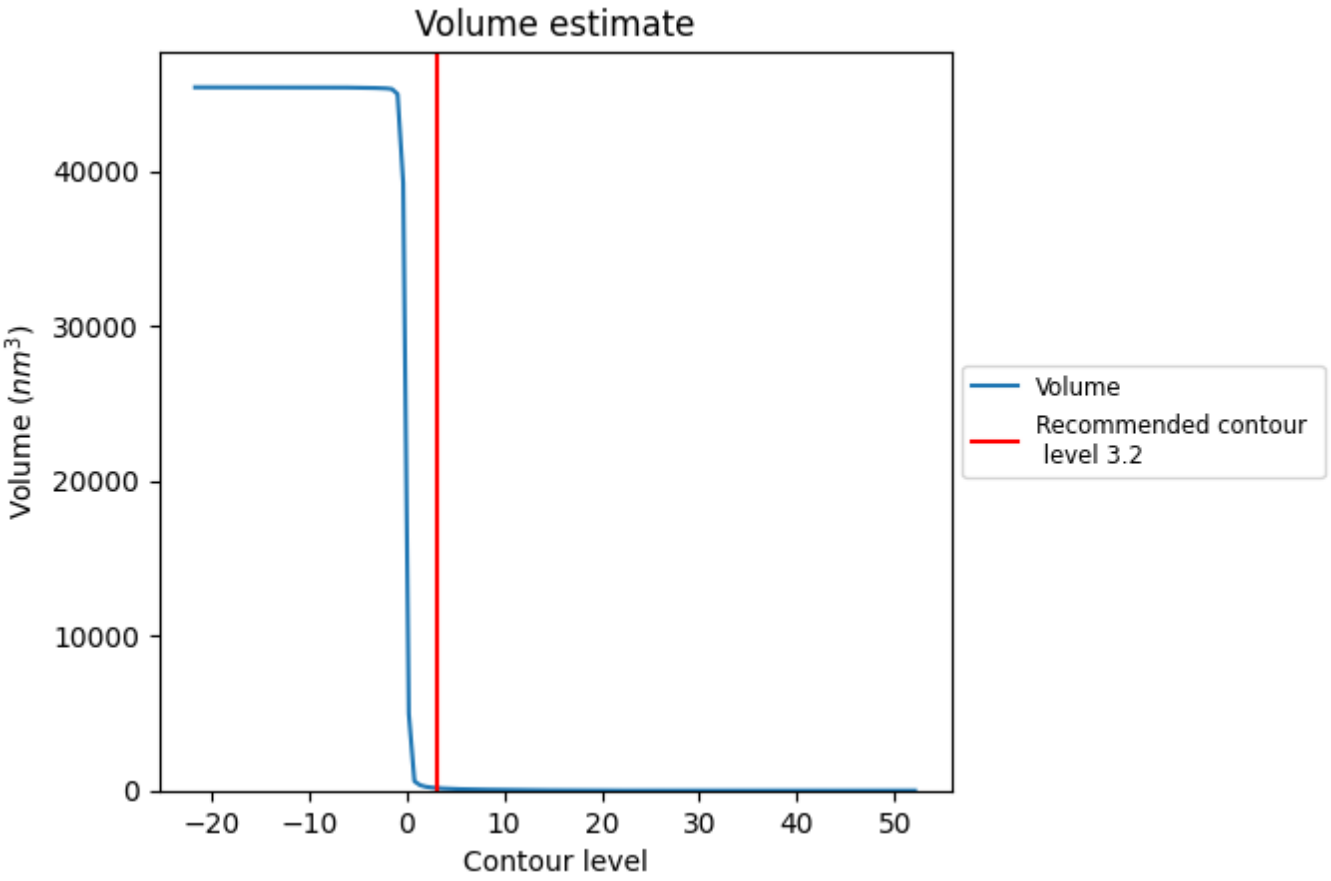
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

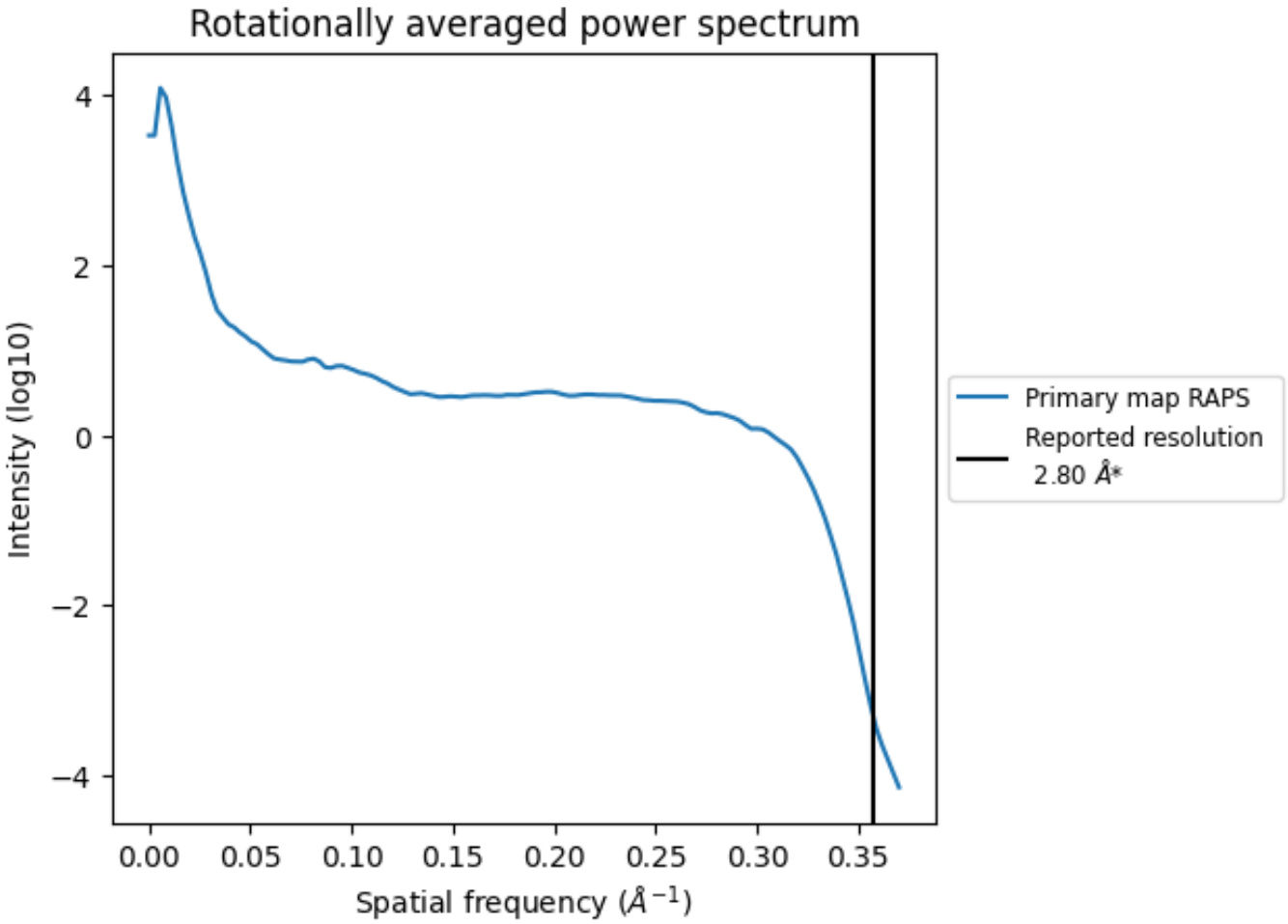
7.2 Volume estimate



The volume at the recommended contour level is 157 nm^3; this corresponds to an approximate mass of 142 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 0.357 Å^{-1}

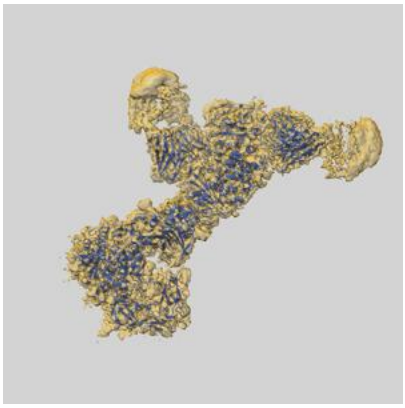
8 Fourier-Shell correlation

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

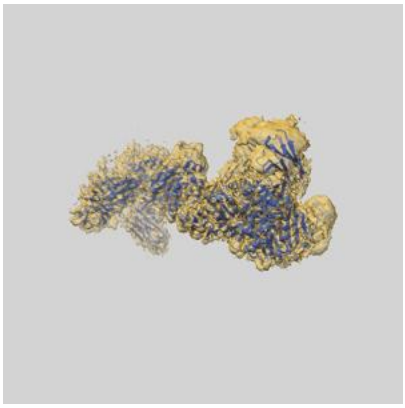
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-23253 and PDB model 7LBF. Per-residue inclusion information can be found in section 3 on page 10.

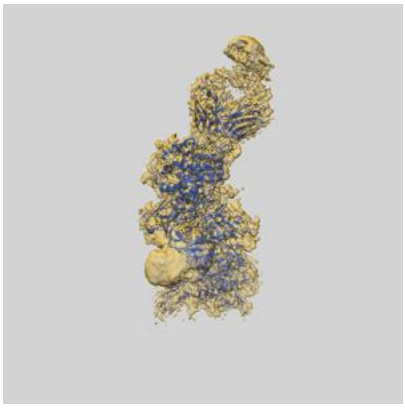
9.1 Map-model overlay



X



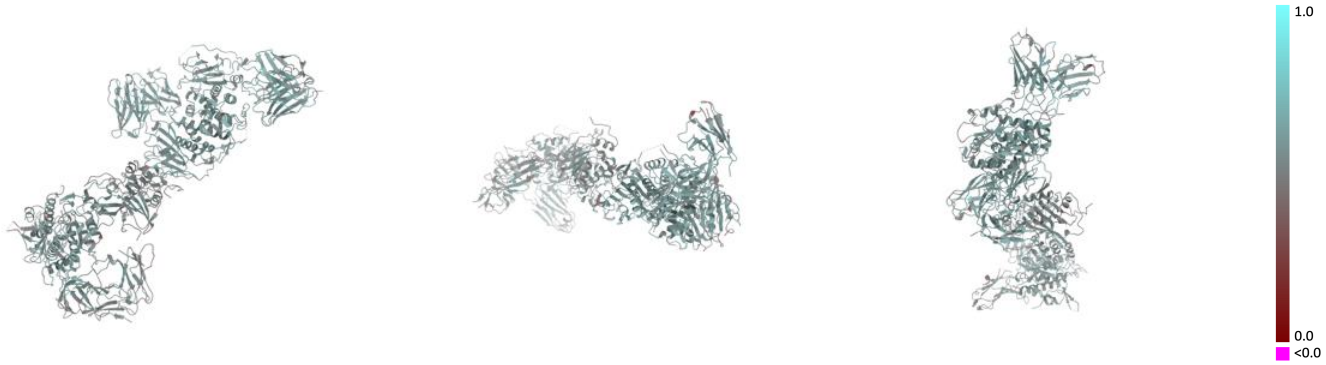
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 3.2 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.

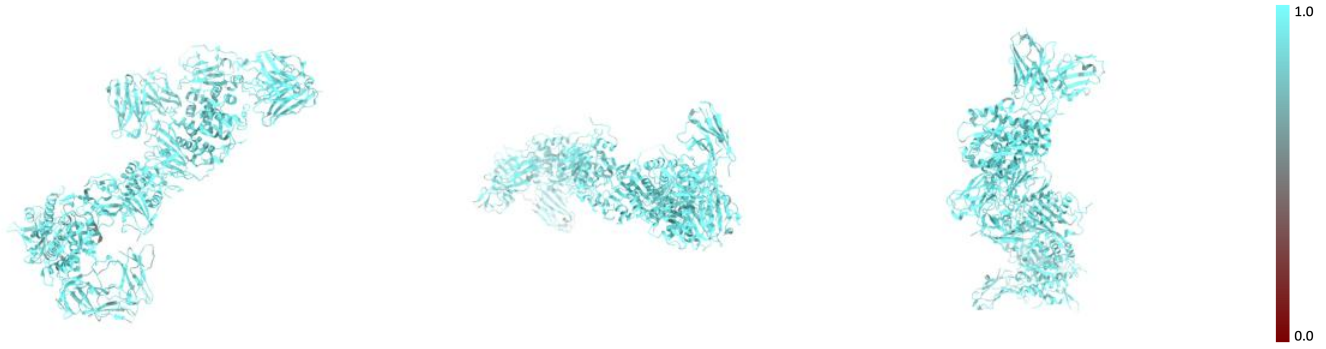
9.2 Q-score mapped to coordinate model (i)



X Y Z

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.

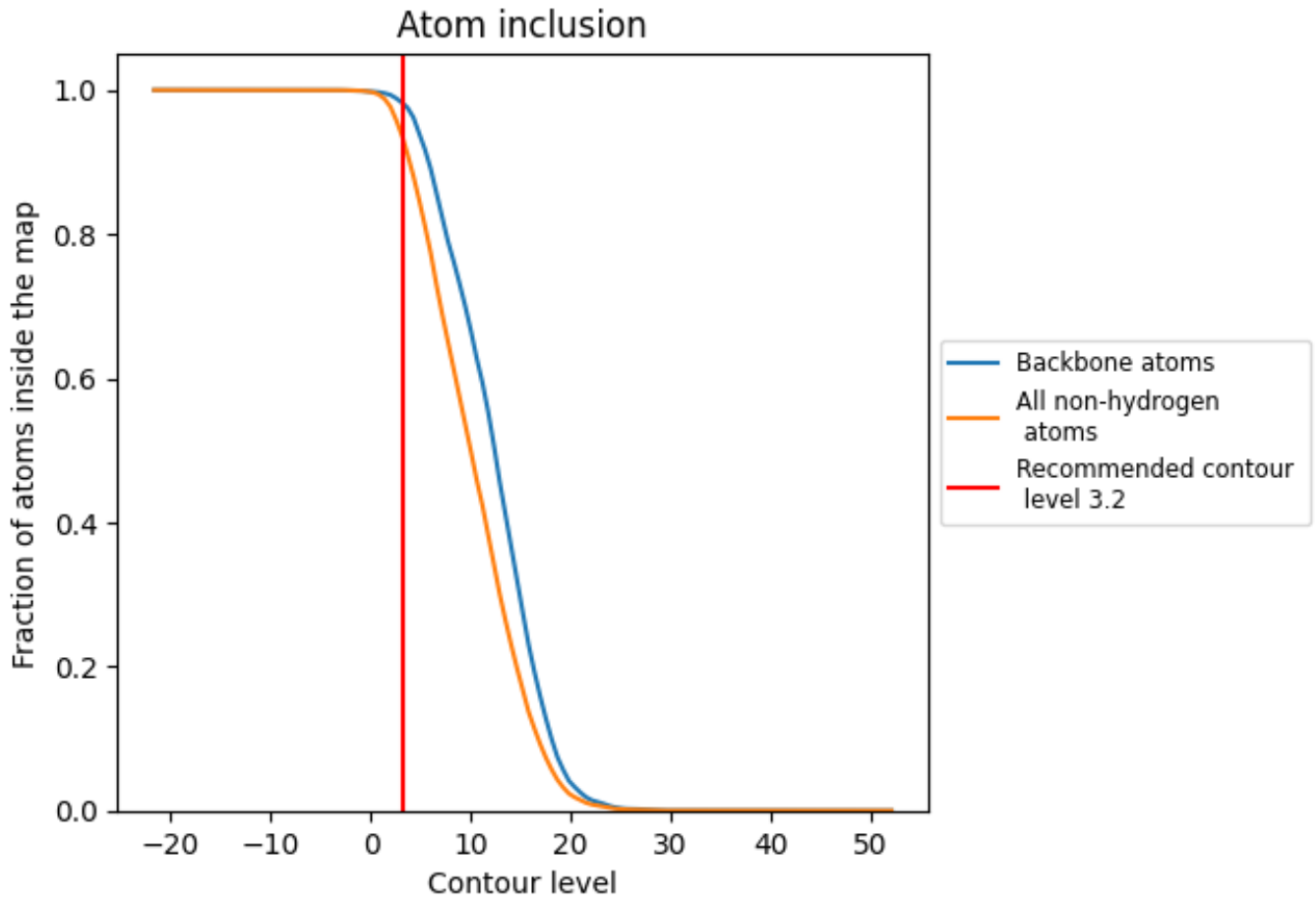
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (3.2).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 93% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (3.2) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9339	0.5480
A	0.9517	0.5600
B	0.9555	0.5250
C	0.9476	0.5450
D	0.8529	0.5070
E	0.9490	0.5750
F	0.9382	0.5760
G	0.9280	0.5590
H	0.9291	0.5740
I	0.9643	0.5690
J	0.8571	0.5310
K	0.9639	0.5340