Full wwPDB EM Validation Report (i)

Nov 14, 2022 – 08:57 PM EST

PDB ID	:	7KEX
EMDB ID	:	EMD-22842
Title	:	Ebola virus GP (mucin deleted, Makona strain) bound to antibody Fab EBOV-293
Authors	:	Murin, C.D.; Ward, A.B.
Deposited on	:	2020-10-13
Resolution	:	4.25 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:

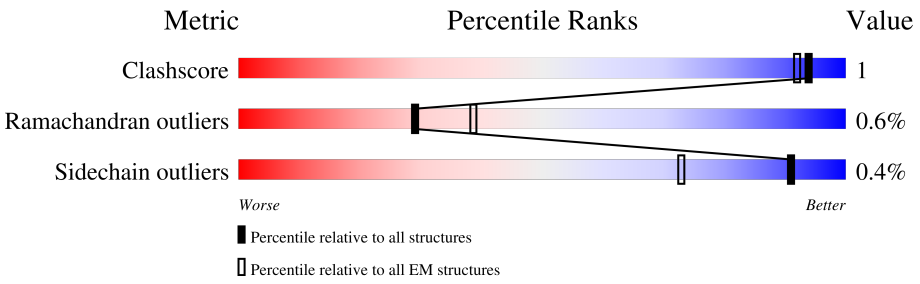
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (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 4.25 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	J	232	44% • 54%
1	K	232	43% • 54%
1	L	232	42% • 54%
2	G	244	45% 5% 50%
2	H	244	45% 5% 50%
2	I	244	45% 5% 50%
3	A	313	63% 7% 30%
3	B	313	63% 7% 30%

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Mol	Chain	Length	Quality of chain
3	C	313	63% 7% 30%
4	D	203	44% 55%
4	E	203	44% 55%
4	F	203	44% 55%
5	M	3	33% 100%
5	O	3	33% 100%
5	Q	3	33% 100%
6	N	4	50% 25% 75%
6	P	4	50% 25% 75%
6	R	4	50% 25% 75%

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 12909 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 Antibody Fab EBOV-293 light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	J	107	812	508	138	163	3	0	0
1	K	107	812	508	138	163	3	0	0
1	L	107	812	508	138	163	3	0	0

- Molecule 2 is a protein called Antibody Fab EBOV-293 heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	G	121	923	588	154	176	5	0	0
2	H	121	923	588	154	176	5	0	0
2	I	121	923	588	154	176	5	0	0

- Molecule 3 is a protein called Virion spike glycoprotein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	A	220	1716	1091	294	326	5	0	0
3	B	220	1716	1091	294	326	5	0	0
3	C	220	1716	1091	294	326	5	0	0

There are 105 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	MET	-	expression tag	UNP A0A1C4HDV6
A	-2	ASP	-	expression tag	UNP A0A1C4HDV6
A	-1	ALA	-	expression tag	UNP A0A1C4HDV6

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Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP A0A1C4HDV6
A	1	LYS	-	expression tag	UNP A0A1C4HDV6
A	2	ARG	-	expression tag	UNP A0A1C4HDV6
A	3	GLY	-	expression tag	UNP A0A1C4HDV6
A	4	LEU	-	expression tag	UNP A0A1C4HDV6
A	5	CYS	-	expression tag	UNP A0A1C4HDV6
A	6	CYS	-	expression tag	UNP A0A1C4HDV6
A	7	VAL	-	expression tag	UNP A0A1C4HDV6
A	8	LEU	-	expression tag	UNP A0A1C4HDV6
A	9	LEU	-	expression tag	UNP A0A1C4HDV6
A	10	LEU	-	expression tag	UNP A0A1C4HDV6
A	11	CYS	-	expression tag	UNP A0A1C4HDV6
A	12	GLY	-	expression tag	UNP A0A1C4HDV6
A	13	ALA	-	expression tag	UNP A0A1C4HDV6
A	14	VAL	-	expression tag	UNP A0A1C4HDV6
A	15	PHE	-	expression tag	UNP A0A1C4HDV6
A	16	VAL	-	expression tag	UNP A0A1C4HDV6
A	17	SER	-	expression tag	UNP A0A1C4HDV6
A	18	PRO	-	expression tag	UNP A0A1C4HDV6
A	19	SER	-	expression tag	UNP A0A1C4HDV6
A	20	GLN	-	expression tag	UNP A0A1C4HDV6
A	21	GLU	-	expression tag	UNP A0A1C4HDV6
A	22	ILE	-	expression tag	UNP A0A1C4HDV6
A	23	HIS	-	expression tag	UNP A0A1C4HDV6
A	24	ALA	-	expression tag	UNP A0A1C4HDV6
A	25	ARG	-	expression tag	UNP A0A1C4HDV6
A	26	PHE	-	expression tag	UNP A0A1C4HDV6
A	27	ARG	-	expression tag	UNP A0A1C4HDV6
A	28	ARG	-	expression tag	UNP A0A1C4HDV6
A	29	GLY	-	expression tag	UNP A0A1C4HDV6
A	30	ALA	-	expression tag	UNP A0A1C4HDV6
A	31	ARG	-	expression tag	UNP A0A1C4HDV6
B	-3	MET	-	expression tag	UNP A0A1C4HDV6
B	-2	ASP	-	expression tag	UNP A0A1C4HDV6
B	-1	ALA	-	expression tag	UNP A0A1C4HDV6
B	0	MET	-	expression tag	UNP A0A1C4HDV6
B	1	LYS	-	expression tag	UNP A0A1C4HDV6
B	2	ARG	-	expression tag	UNP A0A1C4HDV6
B	3	GLY	-	expression tag	UNP A0A1C4HDV6
B	4	LEU	-	expression tag	UNP A0A1C4HDV6
B	5	CYS	-	expression tag	UNP A0A1C4HDV6
B	6	CYS	-	expression tag	UNP A0A1C4HDV6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	7	VAL	-	expression tag	UNP A0A1C4HDV6
B	8	LEU	-	expression tag	UNP A0A1C4HDV6
B	9	LEU	-	expression tag	UNP A0A1C4HDV6
B	10	LEU	-	expression tag	UNP A0A1C4HDV6
B	11	CYS	-	expression tag	UNP A0A1C4HDV6
B	12	GLY	-	expression tag	UNP A0A1C4HDV6
B	13	ALA	-	expression tag	UNP A0A1C4HDV6
B	14	VAL	-	expression tag	UNP A0A1C4HDV6
B	15	PHE	-	expression tag	UNP A0A1C4HDV6
B	16	VAL	-	expression tag	UNP A0A1C4HDV6
B	17	SER	-	expression tag	UNP A0A1C4HDV6
B	18	PRO	-	expression tag	UNP A0A1C4HDV6
B	19	SER	-	expression tag	UNP A0A1C4HDV6
B	20	GLN	-	expression tag	UNP A0A1C4HDV6
B	21	GLU	-	expression tag	UNP A0A1C4HDV6
B	22	ILE	-	expression tag	UNP A0A1C4HDV6
B	23	HIS	-	expression tag	UNP A0A1C4HDV6
B	24	ALA	-	expression tag	UNP A0A1C4HDV6
B	25	ARG	-	expression tag	UNP A0A1C4HDV6
B	26	PHE	-	expression tag	UNP A0A1C4HDV6
B	27	ARG	-	expression tag	UNP A0A1C4HDV6
B	28	ARG	-	expression tag	UNP A0A1C4HDV6
B	29	GLY	-	expression tag	UNP A0A1C4HDV6
B	30	ALA	-	expression tag	UNP A0A1C4HDV6
B	31	ARG	-	expression tag	UNP A0A1C4HDV6
C	-3	MET	-	expression tag	UNP A0A1C4HDV6
C	-2	ASP	-	expression tag	UNP A0A1C4HDV6
C	-1	ALA	-	expression tag	UNP A0A1C4HDV6
C	0	MET	-	expression tag	UNP A0A1C4HDV6
C	1	LYS	-	expression tag	UNP A0A1C4HDV6
C	2	ARG	-	expression tag	UNP A0A1C4HDV6
C	3	GLY	-	expression tag	UNP A0A1C4HDV6
C	4	LEU	-	expression tag	UNP A0A1C4HDV6
C	5	CYS	-	expression tag	UNP A0A1C4HDV6
C	6	CYS	-	expression tag	UNP A0A1C4HDV6
C	7	VAL	-	expression tag	UNP A0A1C4HDV6
C	8	LEU	-	expression tag	UNP A0A1C4HDV6
C	9	LEU	-	expression tag	UNP A0A1C4HDV6
C	10	LEU	-	expression tag	UNP A0A1C4HDV6
C	11	CYS	-	expression tag	UNP A0A1C4HDV6
C	12	GLY	-	expression tag	UNP A0A1C4HDV6
C	13	ALA	-	expression tag	UNP A0A1C4HDV6

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Chain	Residue	Modelled	Actual	Comment	Reference
C	14	VAL	-	expression tag	UNP A0A1C4HDV6
C	15	PHE	-	expression tag	UNP A0A1C4HDV6
C	16	VAL	-	expression tag	UNP A0A1C4HDV6
C	17	SER	-	expression tag	UNP A0A1C4HDV6
C	18	PRO	-	expression tag	UNP A0A1C4HDV6
C	19	SER	-	expression tag	UNP A0A1C4HDV6
C	20	GLN	-	expression tag	UNP A0A1C4HDV6
C	21	GLU	-	expression tag	UNP A0A1C4HDV6
C	22	ILE	-	expression tag	UNP A0A1C4HDV6
C	23	HIS	-	expression tag	UNP A0A1C4HDV6
C	24	ALA	-	expression tag	UNP A0A1C4HDV6
C	25	ARG	-	expression tag	UNP A0A1C4HDV6
C	26	PHE	-	expression tag	UNP A0A1C4HDV6
C	27	ARG	-	expression tag	UNP A0A1C4HDV6
C	28	ARG	-	expression tag	UNP A0A1C4HDV6
C	29	GLY	-	expression tag	UNP A0A1C4HDV6
C	30	ALA	-	expression tag	UNP A0A1C4HDV6
C	31	ARG	-	expression tag	UNP A0A1C4HDV6

- Molecule 4 is a protein called Virion spike glycoprotein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	92	735	474	129	129	3	0	0
			Total	C	N	O	S		
4	E	92	735	474	129	129	3	0	0
			Total	C	N	O	S		
4	F	92	735	474	129	129	3	0	0

There are 102 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	630	ASP	-	expression tag	UNP A0A0E3XK95
D	631	ASP	-	expression tag	UNP A0A0E3XK95
D	632	ASP	-	expression tag	UNP A0A0E3XK95
D	633	LYS	-	expression tag	UNP A0A0E3XK95
D	634	ALA	-	expression tag	UNP A0A0E3XK95
D	635	GLY	-	expression tag	UNP A0A0E3XK95
D	636	TRP	-	expression tag	UNP A0A0E3XK95
D	637	SER	-	expression tag	UNP A0A0E3XK95
D	638	HIS	-	expression tag	UNP A0A0E3XK95
D	639	PRO	-	expression tag	UNP A0A0E3XK95

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Chain	Residue	Modelled	Actual	Comment	Reference
D	640	GLN	-	expression tag	UNP A0A0E3XK95
D	641	PHE	-	expression tag	UNP A0A0E3XK95
D	642	GLU	-	expression tag	UNP A0A0E3XK95
D	643	LYS	-	expression tag	UNP A0A0E3XK95
D	644	GLY	-	expression tag	UNP A0A0E3XK95
D	645	GLY	-	expression tag	UNP A0A0E3XK95
D	646	GLY	-	expression tag	UNP A0A0E3XK95
D	647	SER	-	expression tag	UNP A0A0E3XK95
D	648	GLY	-	expression tag	UNP A0A0E3XK95
D	649	GLY	-	expression tag	UNP A0A0E3XK95
D	650	GLY	-	expression tag	UNP A0A0E3XK95
D	651	SER	-	expression tag	UNP A0A0E3XK95
D	652	GLY	-	expression tag	UNP A0A0E3XK95
D	653	GLY	-	expression tag	UNP A0A0E3XK95
D	654	GLY	-	expression tag	UNP A0A0E3XK95
D	655	SER	-	expression tag	UNP A0A0E3XK95
D	656	TRP	-	expression tag	UNP A0A0E3XK95
D	657	SER	-	expression tag	UNP A0A0E3XK95
D	658	HIS	-	expression tag	UNP A0A0E3XK95
D	659	PRO	-	expression tag	UNP A0A0E3XK95
D	660	GLN	-	expression tag	UNP A0A0E3XK95
D	661	PHE	-	expression tag	UNP A0A0E3XK95
D	662	GLU	-	expression tag	UNP A0A0E3XK95
D	663	LYS	-	expression tag	UNP A0A0E3XK95
E	630	ASP	-	expression tag	UNP A0A0E3XK95
E	631	ASP	-	expression tag	UNP A0A0E3XK95
E	632	ASP	-	expression tag	UNP A0A0E3XK95
E	633	LYS	-	expression tag	UNP A0A0E3XK95
E	634	ALA	-	expression tag	UNP A0A0E3XK95
E	635	GLY	-	expression tag	UNP A0A0E3XK95
E	636	TRP	-	expression tag	UNP A0A0E3XK95
E	637	SER	-	expression tag	UNP A0A0E3XK95
E	638	HIS	-	expression tag	UNP A0A0E3XK95
E	639	PRO	-	expression tag	UNP A0A0E3XK95
E	640	GLN	-	expression tag	UNP A0A0E3XK95
E	641	PHE	-	expression tag	UNP A0A0E3XK95
E	642	GLU	-	expression tag	UNP A0A0E3XK95
E	643	LYS	-	expression tag	UNP A0A0E3XK95
E	644	GLY	-	expression tag	UNP A0A0E3XK95
E	645	GLY	-	expression tag	UNP A0A0E3XK95
E	646	GLY	-	expression tag	UNP A0A0E3XK95
E	647	SER	-	expression tag	UNP A0A0E3XK95

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Chain	Residue	Modelled	Actual	Comment	Reference
E	648	GLY	-	expression tag	UNP A0A0E3XK95
E	649	GLY	-	expression tag	UNP A0A0E3XK95
E	650	GLY	-	expression tag	UNP A0A0E3XK95
E	651	SER	-	expression tag	UNP A0A0E3XK95
E	652	GLY	-	expression tag	UNP A0A0E3XK95
E	653	GLY	-	expression tag	UNP A0A0E3XK95
E	654	GLY	-	expression tag	UNP A0A0E3XK95
E	655	SER	-	expression tag	UNP A0A0E3XK95
E	656	TRP	-	expression tag	UNP A0A0E3XK95
E	657	SER	-	expression tag	UNP A0A0E3XK95
E	658	HIS	-	expression tag	UNP A0A0E3XK95
E	659	PRO	-	expression tag	UNP A0A0E3XK95
E	660	GLN	-	expression tag	UNP A0A0E3XK95
E	661	PHE	-	expression tag	UNP A0A0E3XK95
E	662	GLU	-	expression tag	UNP A0A0E3XK95
E	663	LYS	-	expression tag	UNP A0A0E3XK95
F	630	ASP	-	expression tag	UNP A0A0E3XK95
F	631	ASP	-	expression tag	UNP A0A0E3XK95
F	632	ASP	-	expression tag	UNP A0A0E3XK95
F	633	LYS	-	expression tag	UNP A0A0E3XK95
F	634	ALA	-	expression tag	UNP A0A0E3XK95
F	635	GLY	-	expression tag	UNP A0A0E3XK95
F	636	TRP	-	expression tag	UNP A0A0E3XK95
F	637	SER	-	expression tag	UNP A0A0E3XK95
F	638	HIS	-	expression tag	UNP A0A0E3XK95
F	639	PRO	-	expression tag	UNP A0A0E3XK95
F	640	GLN	-	expression tag	UNP A0A0E3XK95
F	641	PHE	-	expression tag	UNP A0A0E3XK95
F	642	GLU	-	expression tag	UNP A0A0E3XK95
F	643	LYS	-	expression tag	UNP A0A0E3XK95
F	644	GLY	-	expression tag	UNP A0A0E3XK95
F	645	GLY	-	expression tag	UNP A0A0E3XK95
F	646	GLY	-	expression tag	UNP A0A0E3XK95
F	647	SER	-	expression tag	UNP A0A0E3XK95
F	648	GLY	-	expression tag	UNP A0A0E3XK95
F	649	GLY	-	expression tag	UNP A0A0E3XK95
F	650	GLY	-	expression tag	UNP A0A0E3XK95
F	651	SER	-	expression tag	UNP A0A0E3XK95
F	652	GLY	-	expression tag	UNP A0A0E3XK95
F	653	GLY	-	expression tag	UNP A0A0E3XK95
F	654	GLY	-	expression tag	UNP A0A0E3XK95
F	655	SER	-	expression tag	UNP A0A0E3XK95

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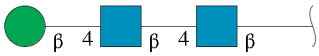
Chain	Residue	Modelled	Actual	Comment	Reference
F	656	TRP	-	expression tag	UNP A0A0E3XK95
F	657	SER	-	expression tag	UNP A0A0E3XK95
F	658	HIS	-	expression tag	UNP A0A0E3XK95
F	659	PRO	-	expression tag	UNP A0A0E3XK95
F	660	GLN	-	expression tag	UNP A0A0E3XK95
F	661	PHE	-	expression tag	UNP A0A0E3XK95
F	662	GLU	-	expression tag	UNP A0A0E3XK95
F	663	LYS	-	expression tag	UNP A0A0E3XK95

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

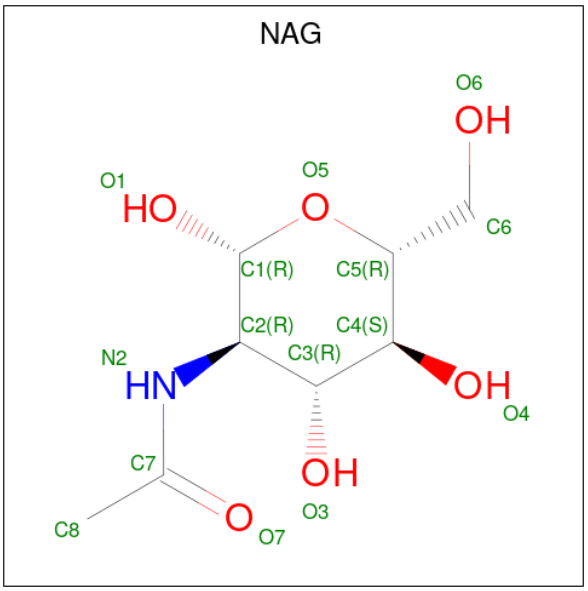


Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
5	M	3	39	22	2	15	0	0
5	O	3	39	22	2	15	0	0
5	Q	3	39	22	2	15	0	0

- Molecule 6 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
			Total	C	N	O		
6	N	4	50	28	2	20	0	0
6	P	4	50	28	2	20	0	0
6	R	4	50	28	2	20	0	0

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



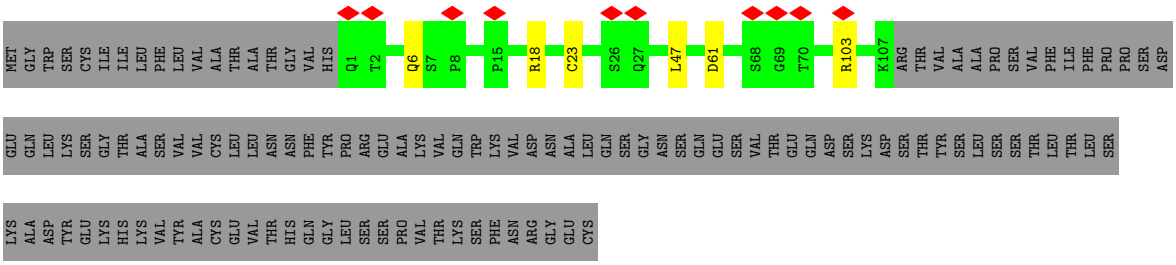
Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
7	A	1	28	16	2	10	0
			Total	C	N	O	
7	A	1	28	16	2	10	0
			Total	C	N	O	
7	B	1	28	16	2	10	0
			Total	C	N	O	
7	B	1	28	16	2	10	0
			Total	C	N	O	
7	C	1	28	16	2	10	0
			Total	C	N	O	
7	C	1	28	16	2	10	0

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.

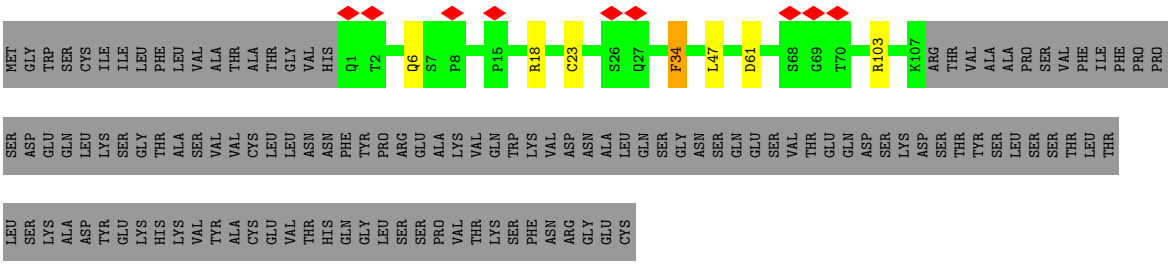
• Molecule 1: Antibody Fab EBOV-293 light chain

Chain J:



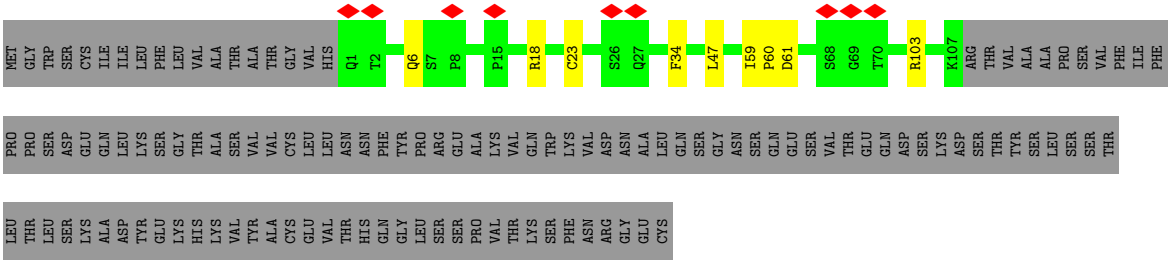
• Molecule 1: Antibody Fab EBOV-293 light chain

Chain K:



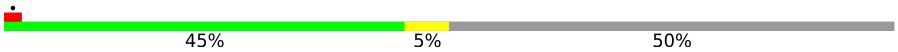
• Molecule 1: Antibody Fab EBOV-293 light chain

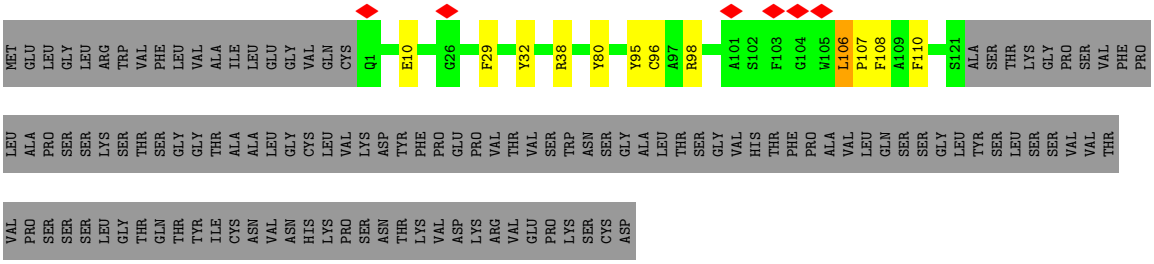
Chain L:



- Molecule 2: Antibody Fab EBOV-293 heavy chain

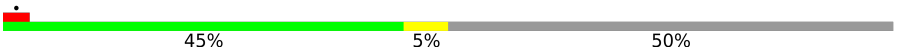
Chain G:

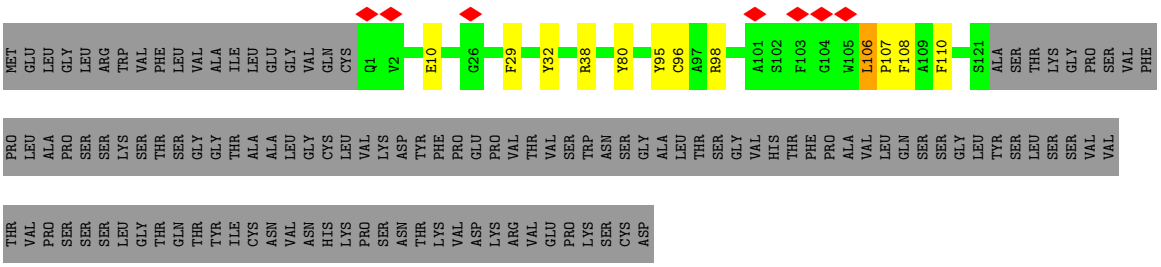




- Molecule 2: Antibody Fab EBOV-293 heavy chain

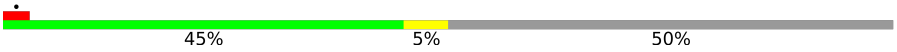
Chain H:

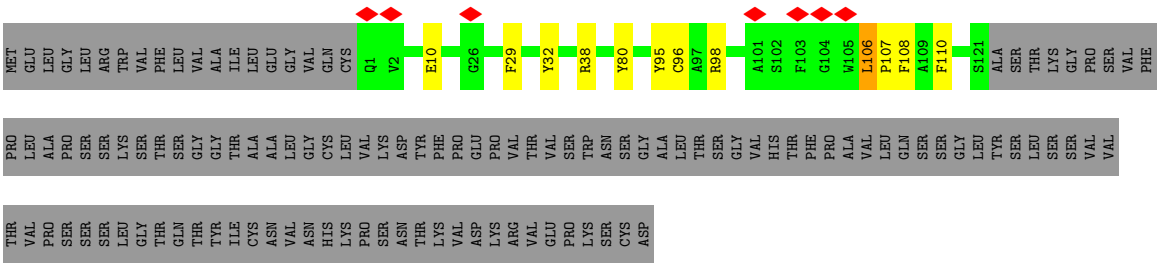




- Molecule 2: Antibody Fab EBOV-293 heavy chain

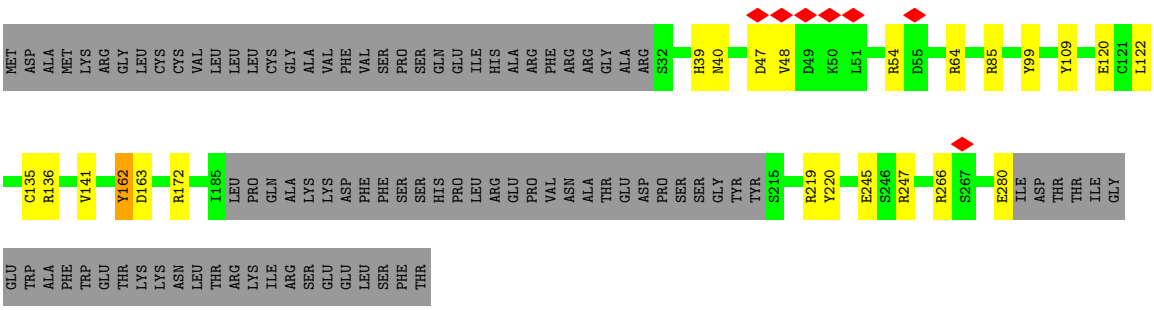
Chain I:





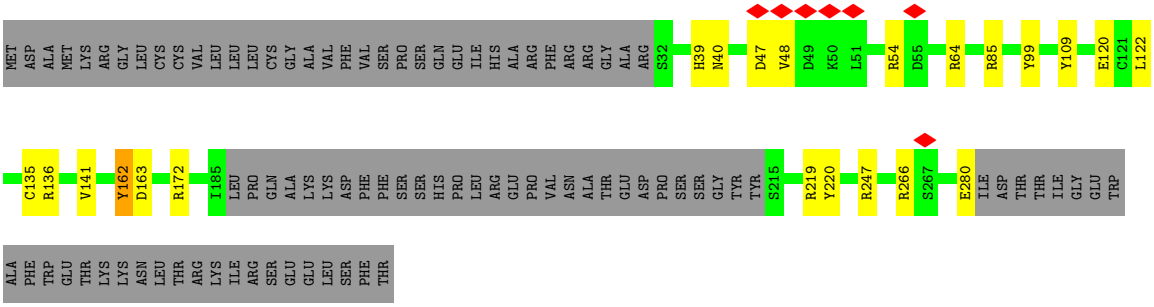
- Molecule 3: Virion spike glycoprotein 1

Chain A:



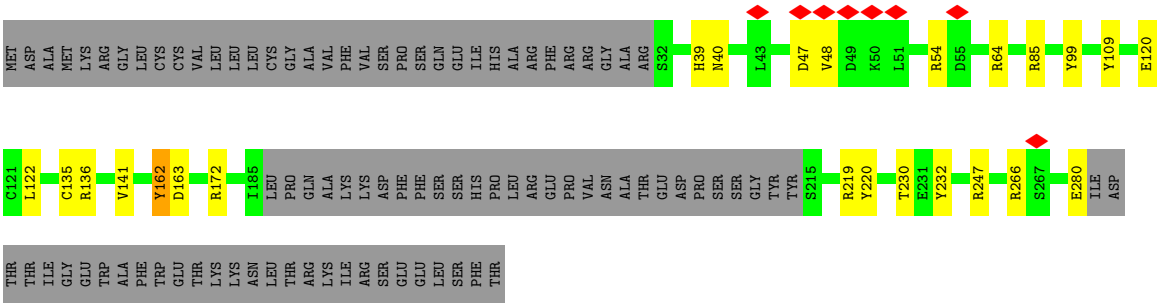
• Molecule 3: Virion spike glycoprotein 1

Chain B:



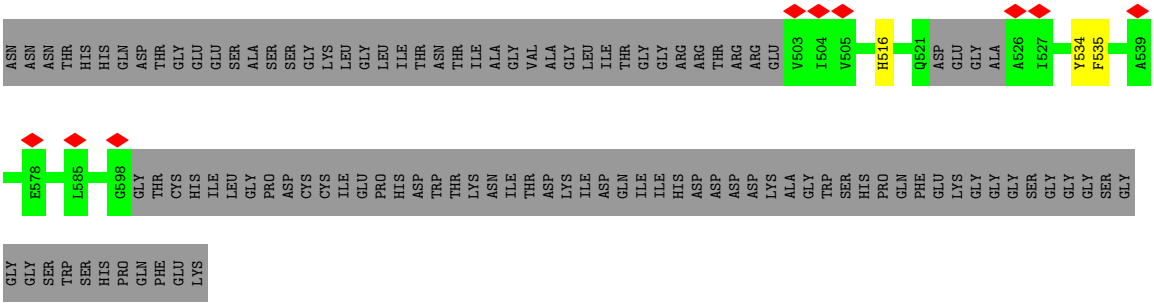
• Molecule 3: Virion spike glycoprotein 1

Chain C:



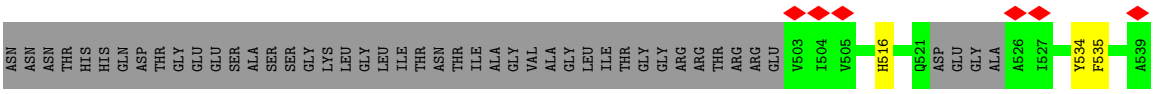
• Molecule 4: Virion spike glycoprotein 2

Chain D:



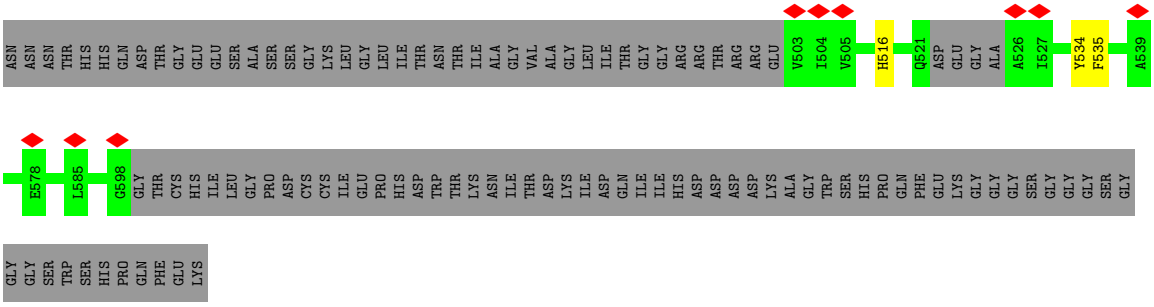
• Molecule 4: Virion spike glycoprotein 2

Chain E:



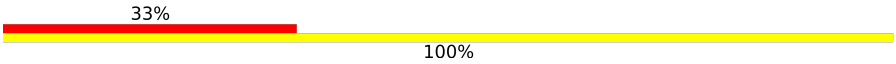
• Molecule 4: Virion spike glycoprotein 2

Chain F:



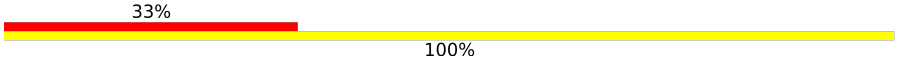
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain M:



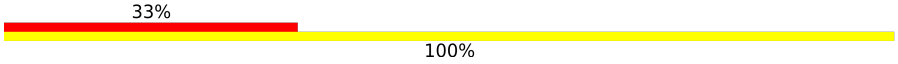
• Molecule 5: beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain O:



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

Chain Q:



• Molecule 6: 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 N:

• Molecule 6: 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 P:

• Molecule 6: 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 R:

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	79722	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	2.399	Depositor
Minimum map value	-0.786	Depositor
Average map value	-0.002	Depositor
Map value standard deviation	0.089	Depositor
Recommended contour level	0.572	Depositor
Map size (Å)	368.0, 368.0, 368.0	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.15, 1.15, 1.15	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: 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	J	1.09	0/830	1.08	2/1126 (0.2%)
1	K	1.09	1/830 (0.1%)	1.08	2/1126 (0.2%)
1	L	1.09	1/830 (0.1%)	1.08	2/1126 (0.2%)
2	G	1.24	8/945 (0.8%)	0.99	2/1284 (0.2%)
2	H	1.24	8/945 (0.8%)	0.99	2/1284 (0.2%)
2	I	1.24	8/945 (0.8%)	0.99	2/1284 (0.2%)
3	A	1.13	5/1755 (0.3%)	1.03	9/2383 (0.4%)
3	B	1.13	4/1755 (0.2%)	1.03	9/2383 (0.4%)
3	C	1.13	4/1755 (0.2%)	1.03	9/2383 (0.4%)
4	D	1.05	1/753 (0.1%)	0.94	1/1026 (0.1%)
4	E	1.05	1/753 (0.1%)	0.94	1/1026 (0.1%)
4	F	1.05	1/753 (0.1%)	0.94	1/1026 (0.1%)
All	All	1.13	42/12849 (0.3%)	1.02	42/17457 (0.2%)

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	108	PHE	CB-CG	-9.01	1.36	1.51
2	G	108	PHE	CB-CG	-8.99	1.36	1.51
2	I	108	PHE	CB-CG	-8.96	1.36	1.51
2	G	95	TYR	CB-CG	-7.91	1.39	1.51
2	I	95	TYR	CB-CG	-7.91	1.39	1.51
2	H	95	TYR	CB-CG	-7.90	1.39	1.51
2	G	96	CYS	CB-SG	-7.29	1.69	1.82
2	I	96	CYS	CB-SG	-7.24	1.70	1.82
2	H	96	CYS	CB-SG	-7.21	1.70	1.82
3	B	99	TYR	CB-CG	-6.98	1.41	1.51
3	A	99	TYR	CB-CG	-6.92	1.41	1.51
3	C	99	TYR	CB-CG	-6.88	1.41	1.51
2	H	80	TYR	CB-CG	-6.60	1.41	1.51
2	G	80	TYR	CB-CG	-6.59	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	80	TYR	CB-CG	-6.59	1.41	1.51
3	B	162	TYR	CB-CG	-6.55	1.41	1.51
3	C	162	TYR	CB-CG	-6.52	1.41	1.51
3	A	162	TYR	CB-CG	-6.51	1.41	1.51
2	G	32	TYR	CB-CG	-6.27	1.42	1.51
2	H	32	TYR	CB-CG	-6.22	1.42	1.51
2	I	32	TYR	CB-CG	-6.17	1.42	1.51
2	G	29	PHE	CB-CG	-5.83	1.41	1.51
2	H	29	PHE	CB-CG	-5.78	1.41	1.51
2	I	29	PHE	CB-CG	-5.76	1.41	1.51
2	G	108	PHE	CD2-CE2	-5.48	1.28	1.39
2	I	108	PHE	CD2-CE2	-5.45	1.28	1.39
2	H	108	PHE	CD2-CE2	-5.43	1.28	1.39
3	C	280	GLU	CB-CG	5.43	1.62	1.52
3	A	280	GLU	CB-CG	5.41	1.62	1.52
3	B	280	GLU	CB-CG	5.41	1.62	1.52
3	A	162	TYR	CG-CD2	-5.27	1.32	1.39
3	C	162	TYR	CG-CD2	-5.21	1.32	1.39
3	B	162	TYR	CG-CD2	-5.20	1.32	1.39
2	I	10	GLU	CD-OE1	-5.17	1.20	1.25
2	G	10	GLU	CD-OE1	-5.11	1.20	1.25
2	H	10	GLU	CD-OE1	-5.09	1.20	1.25
4	F	535	PHE	CB-CG	-5.09	1.42	1.51
4	E	535	PHE	CB-CG	-5.09	1.42	1.51
1	K	34	PHE	CB-CG	-5.06	1.42	1.51
4	D	535	PHE	CB-CG	-5.04	1.42	1.51
1	L	34	PHE	CB-CG	-5.03	1.42	1.51
3	A	245	GLU	CD-OE1	-5.03	1.20	1.25

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	220	TYR	CB-CG-CD1	-9.09	115.54	121.00
3	C	220	TYR	CB-CG-CD1	-9.06	115.56	121.00
3	B	220	TYR	CB-CG-CD1	-8.94	115.64	121.00
3	A	162	TYR	CB-CG-CD2	-7.93	116.24	121.00
3	C	162	TYR	CB-CG-CD2	-7.92	116.25	121.00
3	B	162	TYR	CB-CG-CD2	-7.89	116.27	121.00
1	K	103	ARG	NE-CZ-NH2	-6.99	116.80	120.30
1	J	103	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	L	103	ARG	NE-CZ-NH2	-6.86	116.87	120.30
3	B	266	ARG	NE-CZ-NH2	-6.64	116.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	266	ARG	NE-CZ-NH2	-6.51	117.04	120.30
3	C	266	ARG	NE-CZ-NH2	-6.47	117.07	120.30
3	B	64	ARG	NE-CZ-NH2	-6.45	117.08	120.30
3	A	85	ARG	NE-CZ-NH2	-6.41	117.09	120.30
2	I	95	TYR	CB-CG-CD2	-6.36	117.19	121.00
2	H	95	TYR	CB-CG-CD2	-6.35	117.19	121.00
3	B	85	ARG	NE-CZ-NH2	-6.33	117.14	120.30
3	C	85	ARG	NE-CZ-NH2	-6.32	117.14	120.30
3	C	64	ARG	NE-CZ-NH2	-6.31	117.14	120.30
2	G	95	TYR	CB-CG-CD2	-6.30	117.22	121.00
3	B	247	ARG	NE-CZ-NH2	-6.29	117.16	120.30
3	A	64	ARG	NE-CZ-NH2	-6.28	117.16	120.30
3	C	247	ARG	NE-CZ-NH2	-6.25	117.17	120.30
3	A	247	ARG	NE-CZ-NH2	-6.22	117.19	120.30
3	C	109	TYR	CB-CG-CD1	-6.01	117.39	121.00
3	B	109	TYR	CB-CG-CD1	-5.99	117.41	121.00
3	A	109	TYR	CB-CG-CD1	-5.94	117.44	121.00
2	I	38	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	H	38	ARG	NE-CZ-NH2	-5.50	117.55	120.30
2	G	38	ARG	NE-CZ-NH2	-5.41	117.59	120.30
3	A	54	ARG	NE-CZ-NH1	5.26	122.93	120.30
3	B	54	ARG	NE-CZ-NH1	5.23	122.92	120.30
3	C	54	ARG	NE-CZ-NH1	5.22	122.91	120.30
3	B	219	ARG	NE-CZ-NH2	-5.19	117.70	120.30
3	A	219	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	L	18	ARG	NE-CZ-NH2	-5.06	117.77	120.30
4	E	516	HIS	N-CA-C	-5.05	97.37	111.00
1	J	18	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	K	18	ARG	NE-CZ-NH2	-5.04	117.78	120.30
4	F	516	HIS	N-CA-C	-5.03	97.42	111.00
4	D	516	HIS	N-CA-C	-5.01	97.46	111.00
3	C	219	ARG	NE-CZ-NH2	-5.01	117.79	120.30

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	J	812	0	783	2	0
1	K	812	0	783	3	0
1	L	812	0	783	3	0
2	G	923	0	902	2	0
2	H	923	0	902	2	0
2	I	923	0	902	2	0
3	A	1716	0	1679	5	0
3	B	1716	0	1679	5	0
3	C	1716	0	1679	6	0
4	D	735	0	730	0	0
4	E	735	0	730	0	0
4	F	735	0	730	0	0
5	M	39	0	34	0	0
5	O	39	0	34	0	0
5	Q	39	0	34	0	0
6	N	50	0	43	0	0
6	P	50	0	43	0	0
6	R	50	0	43	0	0
7	A	28	0	26	0	0
7	B	28	0	26	0	0
7	C	28	0	26	0	0
All	All	12909	0	12591	30	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 1.

All (30) 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)
3:B:122:LEU:HB2	3:B:172:ARG:HB2	1.95	0.49
3:A:122:LEU:HB2	3:A:172:ARG:HB2	1.95	0.49
3:C:122:LEU:HB2	3:C:172:ARG:HB2	1.95	0.48
3:C:162:TYR:O	3:C:163:ASP:C	2.52	0.48
3:A:162:TYR:O	3:A:163:ASP:C	2.52	0.47
3:B:162:TYR:O	3:B:163:ASP:C	2.51	0.47
1:J:61:ASP:OD1	1:J:61:ASP:N	2.48	0.46
1:K:61:ASP:OD1	1:K:61:ASP:N	2.48	0.46
2:H:98:ARG:HB3	2:H:110:PHE:HB2	1.99	0.45
2:G:106:LEU:N	2:G:107:PRO:CD	2.80	0.45
1:L:61:ASP:N	1:L:61:ASP:OD1	2.48	0.45
2:I:98:ARG:HB3	2:I:110:PHE:HB2	1.99	0.45
2:I:106:LEU:N	2:I:107:PRO:CD	2.80	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:98:ARG:HB3	2:G:110:PHE:HB2	1.98	0.44
2:H:106:LEU:N	2:H:107:PRO:CD	2.80	0.44
3:A:39:HIS:ND1	3:A:40:ASN:N	2.66	0.43
3:C:39:HIS:ND1	3:C:40:ASN:N	2.66	0.43
3:C:47:ASP:OD1	3:C:48:VAL:N	2.52	0.43
3:B:39:HIS:ND1	3:B:40:ASN:N	2.66	0.42
3:A:47:ASP:OD1	3:A:48:VAL:N	2.52	0.42
1:J:6:GLN:HG2	1:J:23:CYS:SG	2.60	0.42
1:L:6:GLN:HG2	1:L:23:CYS:SG	2.60	0.41
1:K:6:GLN:HG2	1:K:23:CYS:SG	2.60	0.41
1:L:59:ILE:HA	1:L:60:PRO:HD3	1.90	0.41
3:B:47:ASP:OD1	3:B:48:VAL:N	2.52	0.41
3:A:135:CYS:SG	3:A:136:ARG:N	2.94	0.41
3:C:135:CYS:SG	3:C:136:ARG:N	2.94	0.41
3:C:230:THR:HG1	3:C:232:TYR:HE1	1.67	0.40
1:K:34:PHE:CD2	1:K:34:PHE:C	2.95	0.40
3:B:135:CYS:SG	3:B:136:ARG:N	2.94	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	J	105/232 (45%)	102 (97%)	3 (3%)	0	100	100
1	K	105/232 (45%)	102 (97%)	3 (3%)	0	100	100
1	L	105/232 (45%)	102 (97%)	3 (3%)	0	100	100
2	G	119/244 (49%)	116 (98%)	2 (2%)	1 (1%)	19	60
2	H	119/244 (49%)	116 (98%)	2 (2%)	1 (1%)	19	60
2	I	119/244 (49%)	116 (98%)	2 (2%)	1 (1%)	19	60
3	A	216/313 (69%)	205 (95%)	9 (4%)	2 (1%)	17	56

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	B	216/313 (69%)	205 (95%)	9 (4%)	2 (1%)	17	56
3	C	216/313 (69%)	205 (95%)	9 (4%)	2 (1%)	17	56
4	D	90/203 (44%)	88 (98%)	2 (2%)	0	100	100
4	E	90/203 (44%)	88 (98%)	2 (2%)	0	100	100
4	F	90/203 (44%)	88 (98%)	2 (2%)	0	100	100
All	All	1590/2976 (53%)	1533 (96%)	48 (3%)	9 (1%)	29	65

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	120	GLU
3	B	120	GLU
3	C	120	GLU
3	A	141	VAL
3	B	141	VAL
3	C	141	VAL
2	G	106	LEU
2	H	106	LEU
2	I	106	LEU

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	J	89/199 (45%)	88 (99%)	1 (1%)	73	85
1	K	89/199 (45%)	88 (99%)	1 (1%)	73	85
1	L	89/199 (45%)	88 (99%)	1 (1%)	73	85
2	G	98/204 (48%)	98 (100%)	0	100	100
2	H	98/204 (48%)	98 (100%)	0	100	100
2	I	98/204 (48%)	98 (100%)	0	100	100
3	A	187/268 (70%)	187 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	B	187/268 (70%)	187 (100%)	0	100	100
3	C	187/268 (70%)	187 (100%)	0	100	100
4	D	76/162 (47%)	75 (99%)	1 (1%)	69	82
4	E	76/162 (47%)	75 (99%)	1 (1%)	69	82
4	F	76/162 (47%)	75 (99%)	1 (1%)	69	82
All	All	1350/2499 (54%)	1344 (100%)	6 (0%)	91	94

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	J	47	LEU
4	D	534	TYR
1	K	47	LEU
4	E	534	TYR
1	L	47	LEU
4	F	534	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

21 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	M	1	5,3	14,14,15	1.94	6 (42%)	17,19,21	1.27	2 (11%)
5	NAG	M	2	5	14,14,15	2.02	6 (42%)	17,19,21	1.00	2 (11%)
5	BMA	M	3	5	11,11,12	2.04	6 (54%)	15,15,17	0.77	0
6	NAG	N	1	6,4	14,14,15	2.10	6 (42%)	17,19,21	1.20	2 (11%)
6	NAG	N	2	6	14,14,15	1.87	5 (35%)	17,19,21	1.00	1 (5%)
6	BMA	N	3	6	11,11,12	0.66	0	15,15,17	0.82	0
6	MAN	N	4	6	11,11,12	1.98	5 (45%)	15,15,17	0.70	0
5	NAG	O	1	5,3	14,14,15	1.95	5 (35%)	17,19,21	1.26	1 (5%)
5	NAG	O	2	5	14,14,15	2.03	6 (42%)	17,19,21	0.99	2 (11%)
5	BMA	O	3	5	11,11,12	2.04	6 (54%)	15,15,17	0.77	0
6	NAG	P	1	6,4	14,14,15	2.11	6 (42%)	17,19,21	1.18	2 (11%)
6	NAG	P	2	6	14,14,15	1.88	5 (35%)	17,19,21	0.99	1 (5%)
6	BMA	P	3	6	11,11,12	0.66	0	15,15,17	0.83	0
6	MAN	P	4	6	11,11,12	1.99	5 (45%)	15,15,17	0.70	0
5	NAG	Q	1	5,3	14,14,15	1.95	6 (42%)	17,19,21	1.27	1 (5%)
5	NAG	Q	2	5	14,14,15	2.02	6 (42%)	17,19,21	1.00	2 (11%)
5	BMA	Q	3	5	11,11,12	2.04	6 (54%)	15,15,17	0.77	0
6	NAG	R	1	6,4	14,14,15	2.10	6 (42%)	17,19,21	1.19	2 (11%)
6	NAG	R	2	6	14,14,15	1.88	5 (35%)	17,19,21	1.00	1 (5%)
6	BMA	R	3	6	11,11,12	0.65	0	15,15,17	0.83	0
6	MAN	R	4	6	11,11,12	1.98	5 (45%)	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
5	NAG	M	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	M	2	5	-	0/6/23/26	0/1/1/1
5	BMA	M	3	5	-	1/2/19/22	0/1/1/1
6	NAG	N	1	6,4	-	0/6/23/26	0/1/1/1
6	NAG	N	2	6	-	0/6/23/26	0/1/1/1
6	BMA	N	3	6	-	2/2/19/22	0/1/1/1
6	MAN	N	4	6	-	1/2/19/22	0/1/1/1
5	NAG	O	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	O	2	5	-	0/6/23/26	0/1/1/1
5	BMA	O	3	5	-	1/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	P	1	6,4	-	0/6/23/26	0/1/1/1
6	NAG	P	2	6	-	0/6/23/26	0/1/1/1
6	BMA	P	3	6	-	2/2/19/22	0/1/1/1
6	MAN	P	4	6	-	1/2/19/22	0/1/1/1
5	NAG	Q	1	5,3	-	2/6/23/26	0/1/1/1
5	NAG	Q	2	5	-	0/6/23/26	0/1/1/1
5	BMA	Q	3	5	-	1/2/19/22	0/1/1/1
6	NAG	R	1	6,4	-	0/6/23/26	0/1/1/1
6	NAG	R	2	6	-	0/6/23/26	0/1/1/1
6	BMA	R	3	6	-	2/2/19/22	0/1/1/1
6	MAN	R	4	6	-	1/2/19/22	0/1/1/1

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	N	1	NAG	C1-C2	5.12	1.60	1.52
6	P	1	NAG	C1-C2	5.12	1.60	1.52
6	R	1	NAG	C1-C2	5.12	1.60	1.52
5	Q	1	NAG	C1-C2	4.60	1.59	1.52
5	O	1	NAG	C1-C2	4.58	1.59	1.52
5	M	1	NAG	C1-C2	4.54	1.59	1.52
5	O	2	NAG	C1-C2	4.39	1.58	1.52
5	Q	2	NAG	C1-C2	4.39	1.58	1.52
5	M	2	NAG	C1-C2	4.35	1.58	1.52
6	R	2	NAG	C1-C2	4.11	1.58	1.52
6	P	2	NAG	C1-C2	4.05	1.58	1.52
6	N	2	NAG	C1-C2	3.99	1.58	1.52
5	Q	3	BMA	C2-C3	3.50	1.57	1.52
5	M	3	BMA	C2-C3	3.49	1.57	1.52
5	O	3	BMA	C2-C3	3.47	1.57	1.52
6	P	4	MAN	C2-C3	3.16	1.57	1.52
6	N	4	MAN	C2-C3	3.15	1.57	1.52
6	P	4	MAN	O5-C5	3.13	1.49	1.43
6	N	4	MAN	O5-C5	3.13	1.49	1.43
6	R	4	MAN	O5-C5	3.13	1.49	1.43
6	R	4	MAN	C2-C3	3.12	1.57	1.52
5	O	2	NAG	O5-C5	3.10	1.49	1.43
5	M	2	NAG	O5-C5	3.09	1.49	1.43
5	O	3	BMA	O5-C5	3.08	1.49	1.43
5	Q	3	BMA	O5-C5	3.06	1.49	1.43
5	Q	2	NAG	O5-C5	3.05	1.49	1.43
5	M	3	BMA	O5-C5	3.03	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	3	BMA	C1-C2	2.91	1.58	1.52
5	O	3	BMA	C1-C2	2.90	1.58	1.52
6	R	4	MAN	C1-C2	2.90	1.58	1.52
6	P	4	MAN	C1-C2	2.88	1.58	1.52
6	N	4	MAN	C1-C2	2.87	1.58	1.52
5	M	3	BMA	C1-C2	2.87	1.58	1.52
6	P	2	NAG	O5-C5	2.81	1.49	1.43
6	N	2	NAG	O5-C5	2.81	1.49	1.43
6	R	2	NAG	O5-C5	2.79	1.49	1.43
6	P	1	NAG	C3-C2	2.73	1.58	1.52
5	Q	1	NAG	O5-C5	2.71	1.48	1.43
5	M	1	NAG	O5-C5	2.69	1.48	1.43
5	O	1	NAG	O5-C5	2.67	1.48	1.43
6	N	1	NAG	C3-C2	2.66	1.58	1.52
5	Q	2	NAG	C4-C5	2.66	1.58	1.53
6	R	1	NAG	C3-C2	2.64	1.58	1.52
5	O	2	NAG	C4-C5	2.64	1.58	1.53
5	M	2	NAG	C4-C5	2.62	1.58	1.53
6	R	2	NAG	C4-C5	2.62	1.58	1.53
6	P	2	NAG	C4-C5	2.61	1.58	1.53
6	N	2	NAG	C4-C5	2.59	1.58	1.53
6	P	4	MAN	C4-C5	2.57	1.58	1.53
5	M	3	BMA	C4-C5	2.56	1.58	1.53
5	O	3	BMA	C4-C5	2.55	1.58	1.53
5	Q	3	BMA	C4-C5	2.55	1.58	1.53
6	N	4	MAN	C4-C5	2.54	1.58	1.53
6	R	4	MAN	C4-C5	2.54	1.58	1.53
6	R	1	NAG	O5-C1	2.54	1.47	1.43
6	N	1	NAG	O5-C1	2.54	1.47	1.43
6	P	1	NAG	O5-C5	2.51	1.48	1.43
6	P	1	NAG	O5-C1	2.49	1.47	1.43
5	O	1	NAG	C4-C5	2.46	1.58	1.53
6	R	1	NAG	O5-C5	2.44	1.48	1.43
6	P	2	NAG	C3-C2	2.42	1.57	1.52
6	N	1	NAG	C2-N2	2.41	1.50	1.46
6	N	1	NAG	O5-C5	2.41	1.48	1.43
5	Q	1	NAG	C4-C5	2.41	1.58	1.53
5	M	1	NAG	C4-C5	2.40	1.58	1.53
6	P	1	NAG	C2-N2	2.38	1.50	1.46
6	R	2	NAG	C3-C2	2.38	1.57	1.52
6	N	2	NAG	C3-C2	2.37	1.57	1.52
6	R	1	NAG	C2-N2	2.36	1.50	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	O	2	NAG	C3-C2	2.36	1.57	1.52
5	M	2	NAG	C3-C2	2.32	1.57	1.52
5	Q	2	NAG	C3-C2	2.30	1.57	1.52
5	M	2	NAG	C4-C3	2.27	1.58	1.52
5	O	1	NAG	C3-C2	2.27	1.57	1.52
5	Q	2	NAG	C4-C3	2.27	1.58	1.52
5	M	1	NAG	C3-C2	2.26	1.57	1.52
5	O	2	NAG	C4-C3	2.26	1.58	1.52
6	R	2	NAG	C4-C3	2.22	1.58	1.52
6	N	2	NAG	C4-C3	2.22	1.58	1.52
6	P	2	NAG	C4-C3	2.22	1.58	1.52
5	Q	1	NAG	C3-C2	2.21	1.57	1.52
5	O	1	NAG	O5-C1	2.17	1.47	1.43
5	M	3	BMA	O5-C1	2.15	1.47	1.43
5	Q	2	NAG	C2-N2	2.15	1.50	1.46
5	O	2	NAG	C2-N2	2.14	1.50	1.46
6	N	1	NAG	C4-C3	2.14	1.57	1.52
6	R	1	NAG	C4-C3	2.14	1.57	1.52
5	M	2	NAG	C2-N2	2.12	1.49	1.46
5	M	1	NAG	O5-C1	2.10	1.47	1.43
6	R	4	MAN	C4-C3	2.10	1.57	1.52
5	Q	1	NAG	O5-C1	2.09	1.47	1.43
6	P	4	MAN	C4-C3	2.08	1.57	1.52
5	Q	3	BMA	O5-C1	2.08	1.47	1.43
6	P	1	NAG	C4-C3	2.08	1.57	1.52
6	N	4	MAN	C4-C3	2.08	1.57	1.52
5	O	3	BMA	C4-C3	2.07	1.57	1.52
5	M	3	BMA	C4-C3	2.06	1.57	1.52
5	Q	3	BMA	C4-C3	2.06	1.57	1.52
5	O	3	BMA	O5-C1	2.05	1.47	1.43
5	M	1	NAG	C4-C3	2.05	1.57	1.52
5	Q	1	NAG	C4-C3	2.04	1.57	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	N	1	NAG	C8-C7-N2	3.06	121.27	116.10
6	R	1	NAG	C8-C7-N2	3.02	121.22	116.10
6	P	1	NAG	C8-C7-N2	2.97	121.13	116.10
5	Q	1	NAG	O4-C4-C3	-2.80	103.88	110.35
5	M	1	NAG	O4-C4-C3	-2.80	103.88	110.35
5	O	1	NAG	O4-C4-C3	-2.79	103.91	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	M	2	NAG	C8-C7-N2	2.74	120.74	116.10
5	Q	2	NAG	C8-C7-N2	2.74	120.74	116.10
5	O	2	NAG	C8-C7-N2	2.67	120.62	116.10
6	N	1	NAG	O7-C7-C8	-2.54	117.34	122.06
6	R	1	NAG	O7-C7-C8	-2.49	117.43	122.06
6	P	1	NAG	O7-C7-C8	-2.48	117.45	122.06
5	M	2	NAG	O7-C7-C8	-2.20	117.97	122.06
5	Q	2	NAG	O7-C7-C8	-2.20	117.98	122.06
5	O	2	NAG	O7-C7-C8	-2.17	118.02	122.06
5	M	1	NAG	C8-C7-N2	2.03	119.53	116.10
6	N	2	NAG	C8-C7-N2	2.03	119.53	116.10
6	R	2	NAG	C8-C7-N2	2.02	119.52	116.10
6	P	2	NAG	C8-C7-N2	2.00	119.49	116.10

There are no chirality outliers.

All (18) torsion outliers are listed below:

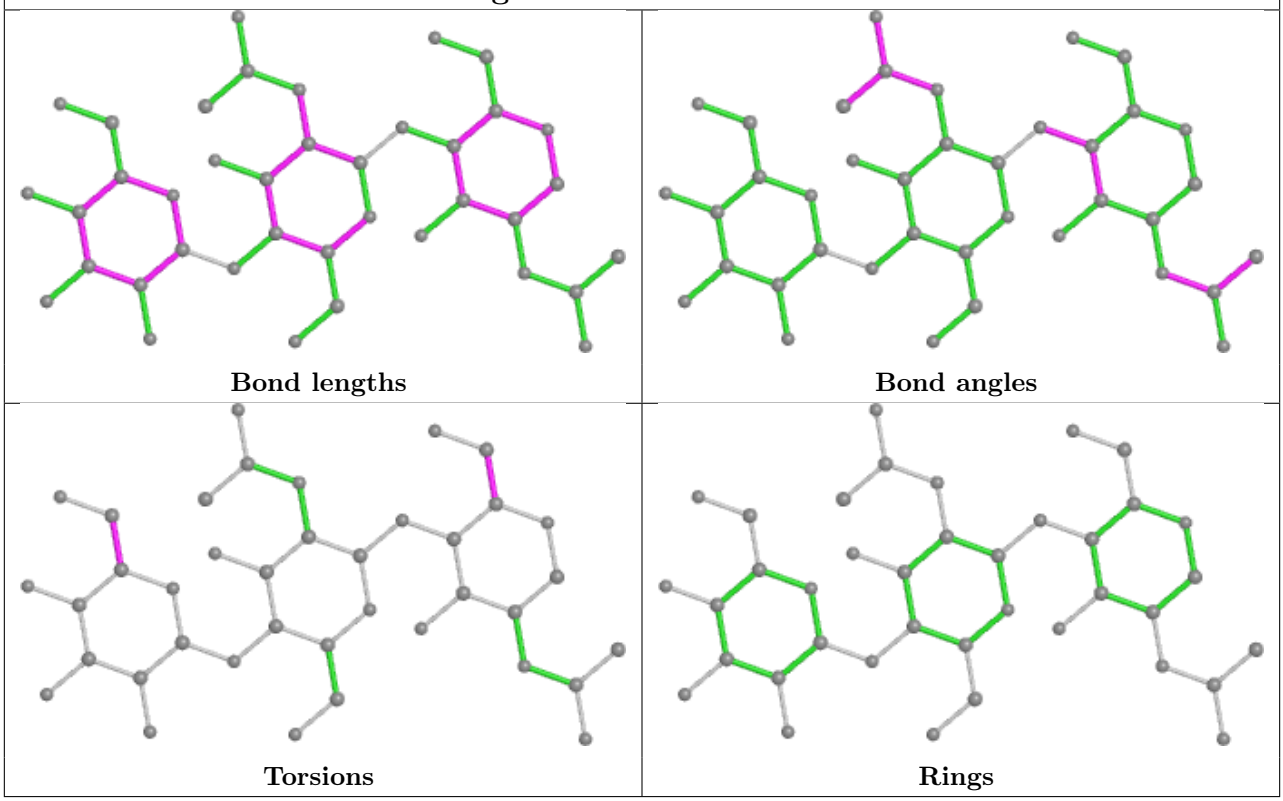
Mol	Chain	Res	Type	Atoms
6	N	3	BMA	C4-C5-C6-O6
6	P	3	BMA	C4-C5-C6-O6
6	R	3	BMA	C4-C5-C6-O6
6	N	3	BMA	O5-C5-C6-O6
6	P	3	BMA	O5-C5-C6-O6
6	R	3	BMA	O5-C5-C6-O6
5	M	3	BMA	O5-C5-C6-O6
5	O	3	BMA	O5-C5-C6-O6
5	Q	3	BMA	O5-C5-C6-O6
6	N	4	MAN	O5-C5-C6-O6
6	P	4	MAN	O5-C5-C6-O6
6	R	4	MAN	O5-C5-C6-O6
5	M	1	NAG	C4-C5-C6-O6
5	O	1	NAG	C4-C5-C6-O6
5	Q	1	NAG	C4-C5-C6-O6
5	M	1	NAG	O5-C5-C6-O6
5	O	1	NAG	O5-C5-C6-O6
5	Q	1	NAG	O5-C5-C6-O6

There are no ring outliers.

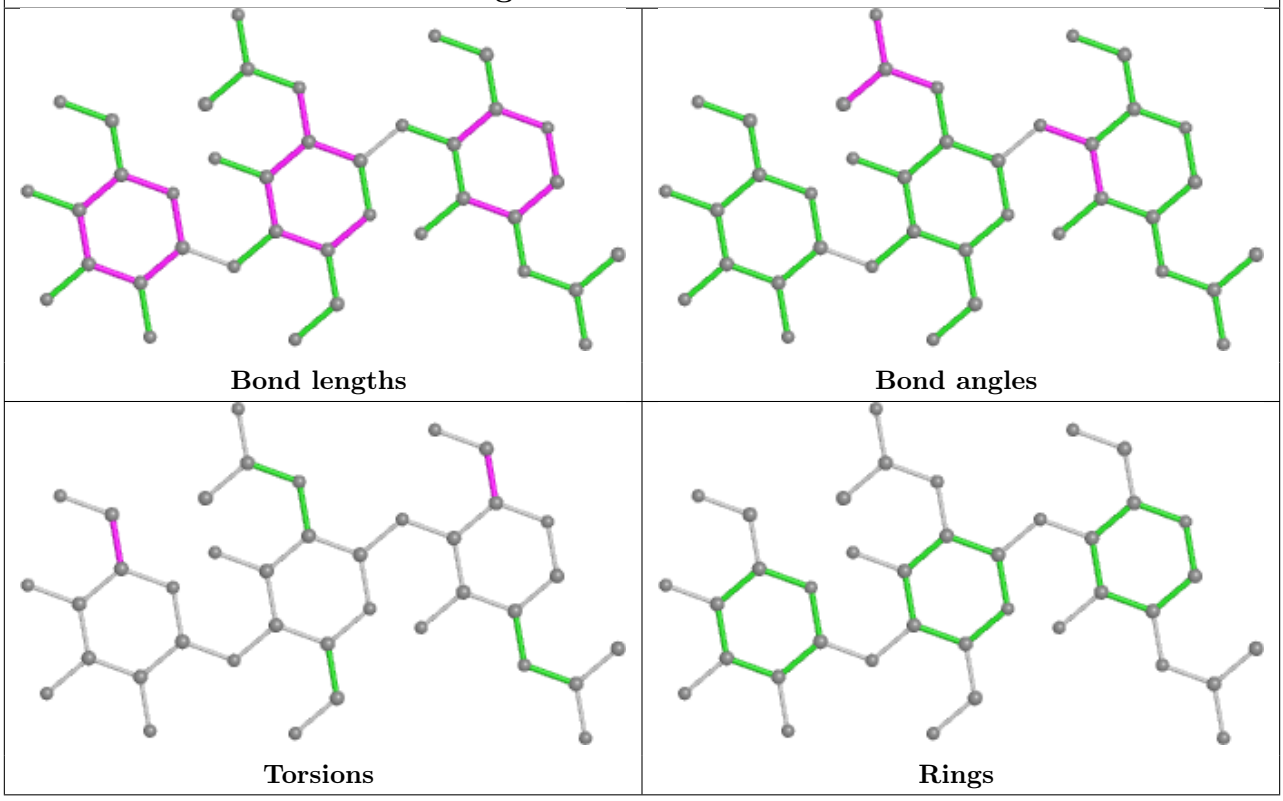
No monomer is involved in short contacts.

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

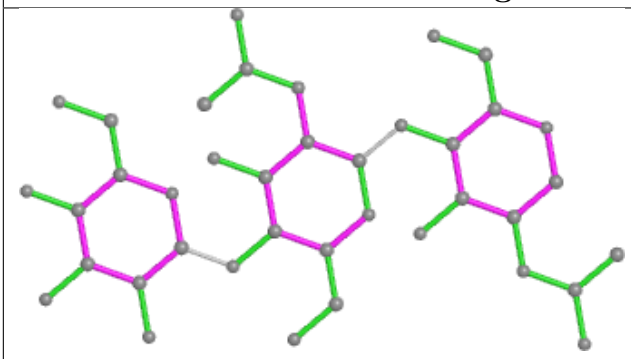
Oligosaccharide Chain M



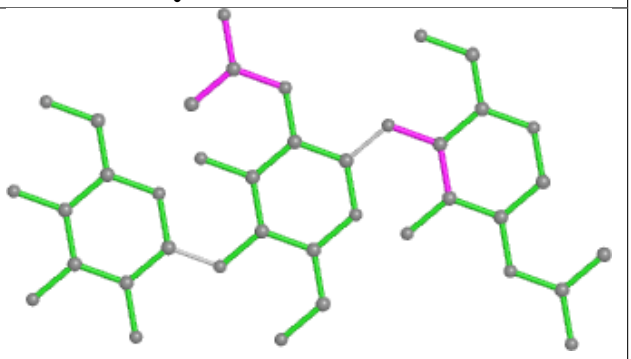
Oligosaccharide Chain O



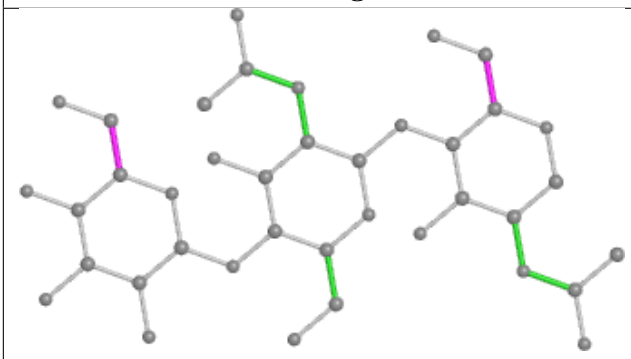
Oligosaccharide Chain Q



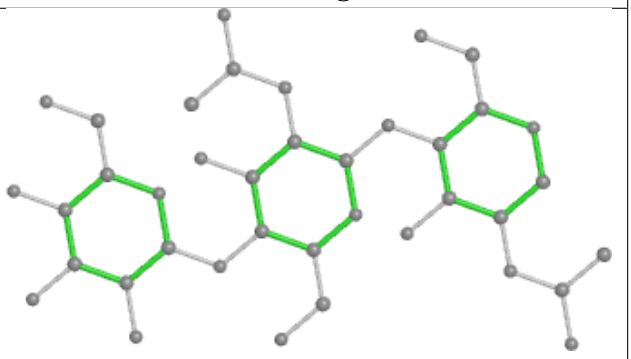
Bond lengths



Bond angles

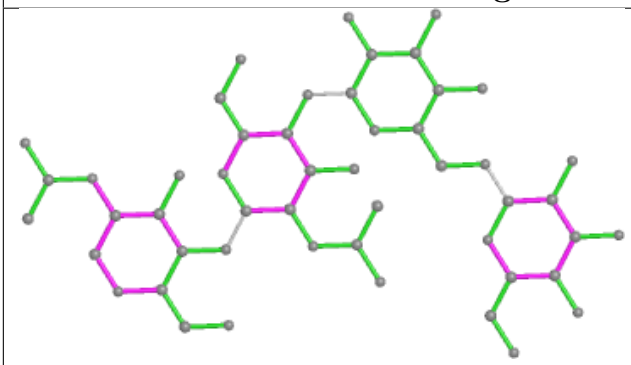


Torsions

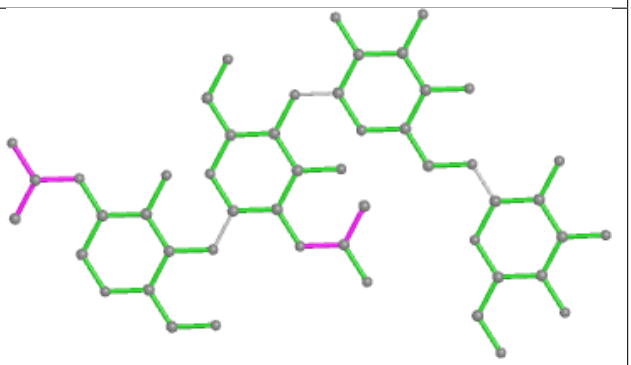


Rings

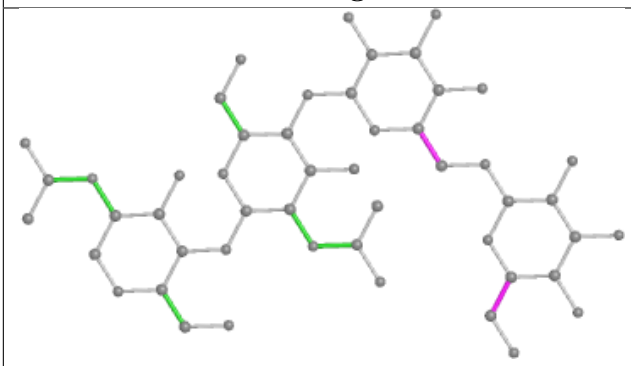
Oligosaccharide Chain N



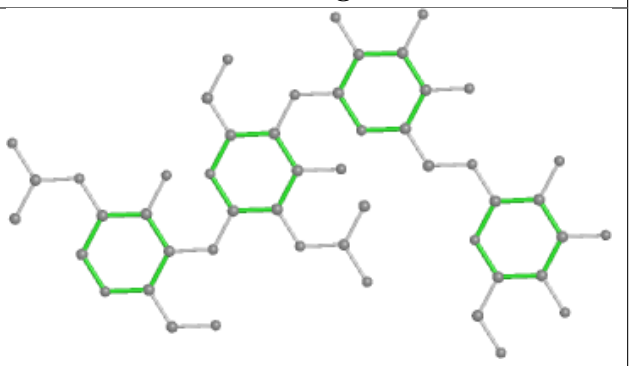
Bond lengths



Bond angles

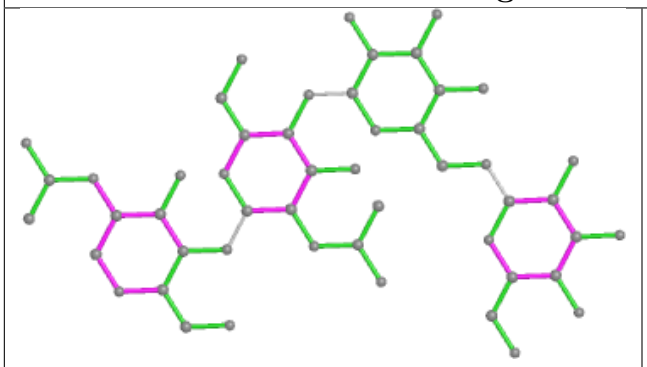


Torsions

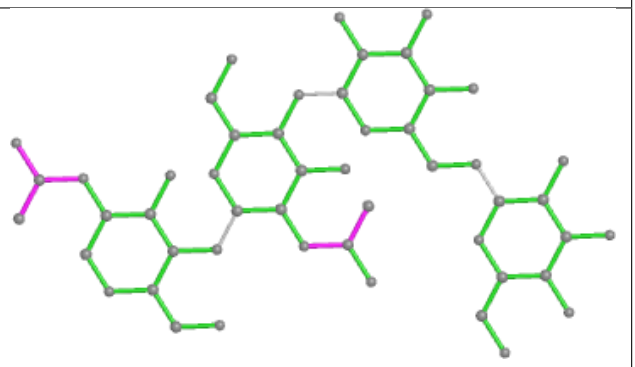


Rings

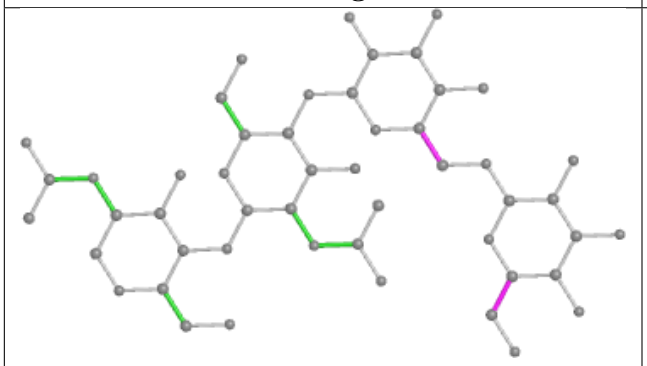
Oligosaccharide Chain P



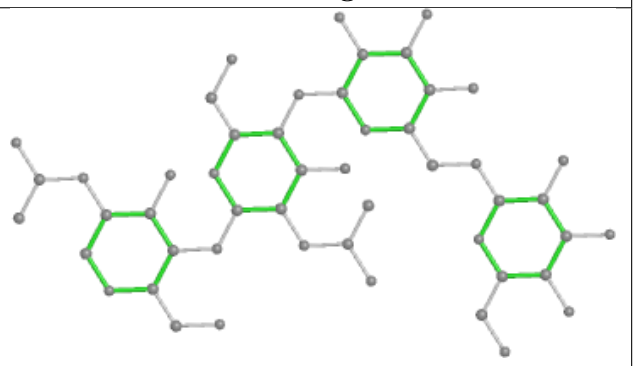
Bond lengths



Bond angles

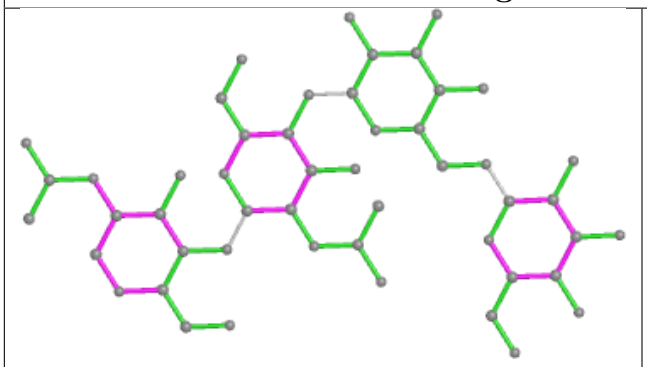


Torsions

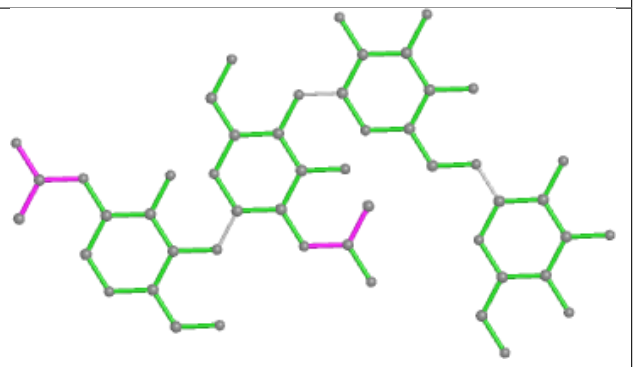


Rings

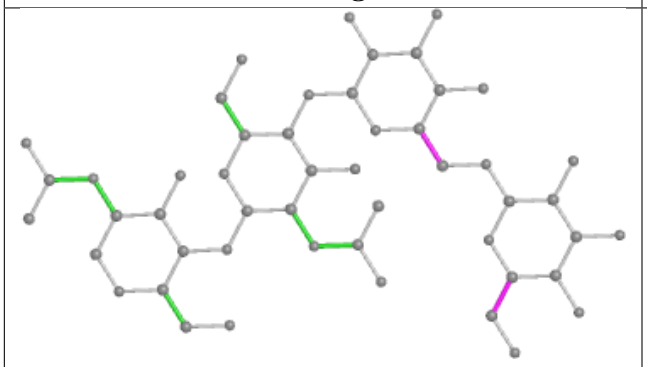
Oligosaccharide Chain R



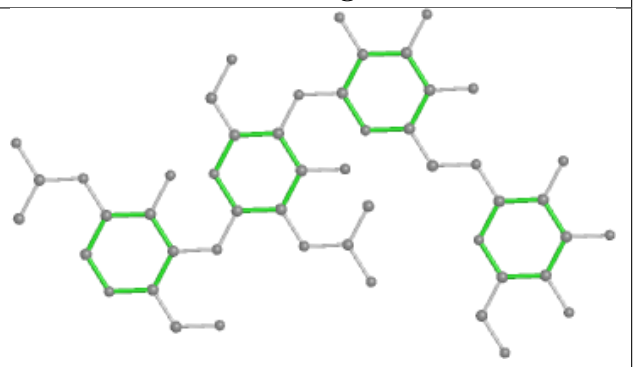
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

6 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	B	402	3	14,14,15	2.19	7 (50%)	17,19,21	0.95	1 (5%)
7	NAG	C	401	3	14,14,15	2.17	7 (50%)	17,19,21	1.01	1 (5%)
7	NAG	B	401	3	14,14,15	2.18	6 (42%)	17,19,21	1.00	1 (5%)
7	NAG	A	401	3	14,14,15	2.18	7 (50%)	17,19,21	1.01	1 (5%)
7	NAG	A	402	3	14,14,15	2.19	7 (50%)	17,19,21	0.95	1 (5%)
7	NAG	C	402	3	14,14,15	2.19	7 (50%)	17,19,21	0.95	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NAG	B	402	3	-	0/6/23/26	0/1/1/1
7	NAG	C	401	3	-	0/6/23/26	0/1/1/1
7	NAG	B	401	3	-	0/6/23/26	0/1/1/1
7	NAG	A	401	3	-	0/6/23/26	0/1/1/1
7	NAG	A	402	3	-	0/6/23/26	0/1/1/1
7	NAG	C	402	3	-	0/6/23/26	0/1/1/1

All (41) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	401	NAG	C1-C2	5.30	1.60	1.52
7	B	402	NAG	C1-C2	5.28	1.60	1.52
7	C	401	NAG	C1-C2	5.25	1.60	1.52
7	C	402	NAG	C1-C2	5.24	1.60	1.52
7	A	402	NAG	C1-C2	5.23	1.60	1.52
7	A	401	NAG	C1-C2	5.21	1.60	1.52
7	B	401	NAG	O5-C5	3.25	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	401	NAG	O5-C5	3.24	1.50	1.43
7	C	401	NAG	O5-C5	3.23	1.50	1.43
7	A	402	NAG	O5-C5	3.13	1.49	1.43
7	C	402	NAG	O5-C5	3.12	1.49	1.43
7	B	402	NAG	O5-C5	3.10	1.49	1.43
7	A	401	NAG	O5-C1	2.84	1.48	1.43
7	B	401	NAG	O5-C1	2.82	1.48	1.43
7	C	401	NAG	O5-C1	2.77	1.48	1.43
7	B	402	NAG	O5-C1	2.76	1.48	1.43
7	A	402	NAG	O5-C1	2.72	1.48	1.43
7	C	402	NAG	O5-C1	2.71	1.48	1.43
7	C	402	NAG	C3-C2	2.43	1.57	1.52
7	A	402	NAG	C3-C2	2.41	1.57	1.52
7	B	402	NAG	C3-C2	2.40	1.57	1.52
7	B	402	NAG	C2-N2	2.37	1.50	1.46
7	A	401	NAG	C4-C5	2.34	1.58	1.53
7	C	402	NAG	C4-C5	2.32	1.57	1.53
7	B	401	NAG	C3-C2	2.31	1.57	1.52
7	A	402	NAG	C2-N2	2.31	1.50	1.46
7	A	402	NAG	C4-C5	2.31	1.57	1.53
7	A	401	NAG	C3-C2	2.31	1.57	1.52
7	C	402	NAG	C2-N2	2.30	1.50	1.46
7	C	401	NAG	C3-C2	2.30	1.57	1.52
7	B	401	NAG	C4-C5	2.29	1.57	1.53
7	B	402	NAG	C4-C5	2.27	1.57	1.53
7	C	401	NAG	C4-C5	2.24	1.57	1.53
7	A	401	NAG	C2-N2	2.15	1.50	1.46
7	B	401	NAG	C2-N2	2.12	1.49	1.46
7	C	402	NAG	C4-C3	2.11	1.57	1.52
7	A	402	NAG	C4-C3	2.11	1.57	1.52
7	C	401	NAG	C2-N2	2.10	1.49	1.46
7	B	402	NAG	C4-C3	2.05	1.57	1.52
7	C	401	NAG	C4-C3	2.05	1.57	1.52
7	A	401	NAG	C4-C3	2.00	1.57	1.52

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	C	401	NAG	C8-C7-N2	2.63	120.55	116.10
7	B	401	NAG	C8-C7-N2	2.62	120.53	116.10
7	A	401	NAG	C8-C7-N2	2.62	120.53	116.10
7	A	402	NAG	C8-C7-N2	2.24	119.89	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	B	402	NAG	C8-C7-N2	2.22	119.86	116.10
7	C	402	NAG	C8-C7-N2	2.21	119.84	116.10

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.

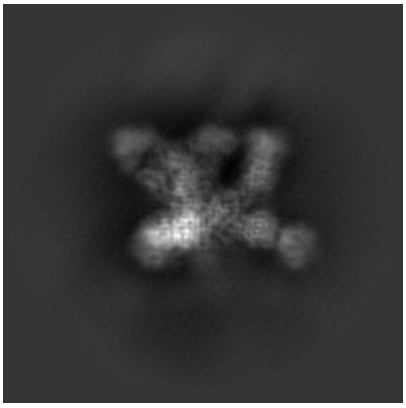
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-22842. These allow visual inspection of the internal detail of the map and identification of artifacts.

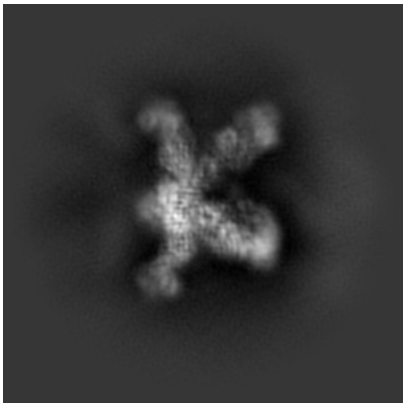
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

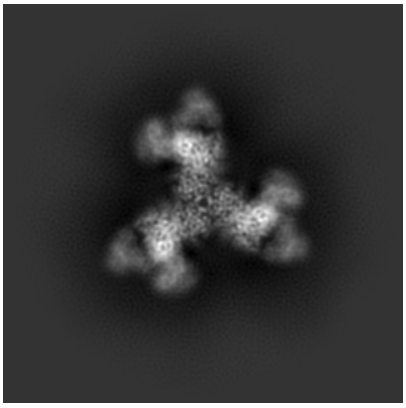
6.1.1 Primary map



X



Y

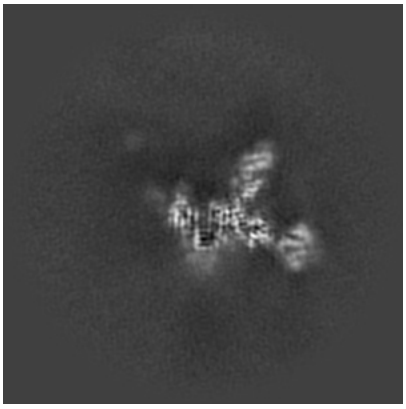


Z

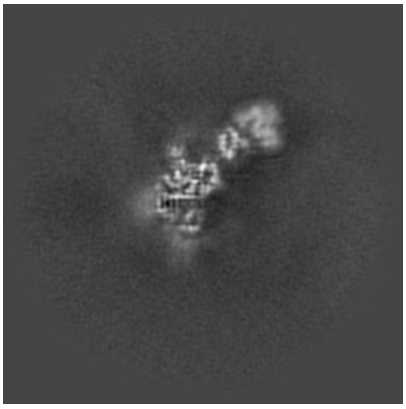
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

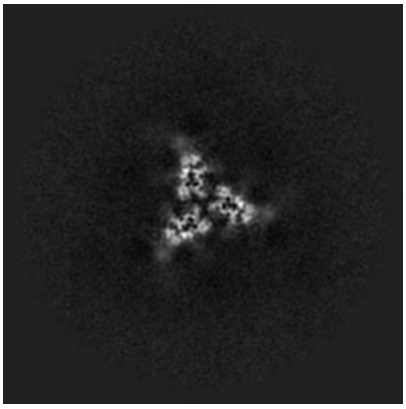
6.2.1 Primary map



X Index: 160



Y Index: 160

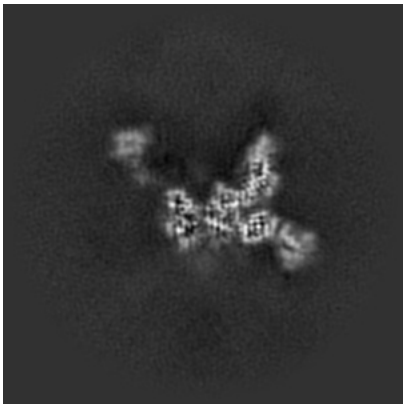


Z Index: 160

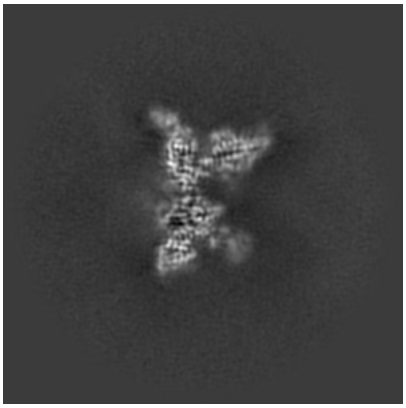
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

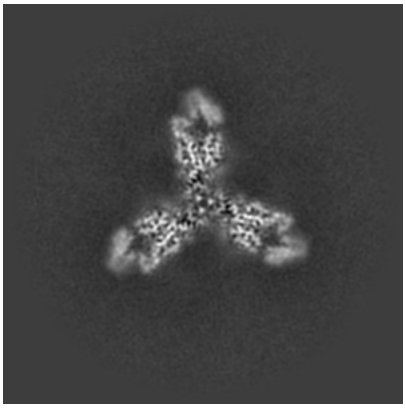
6.3.1 Primary map



X Index: 146



Y Index: 146



Z Index: 137

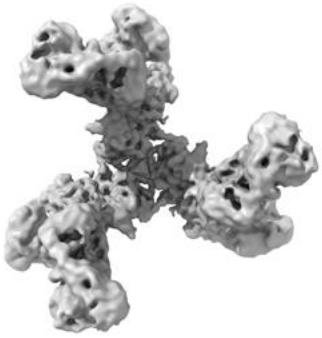
The images above show the largest variance slices of the map in three orthogonal directions.

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

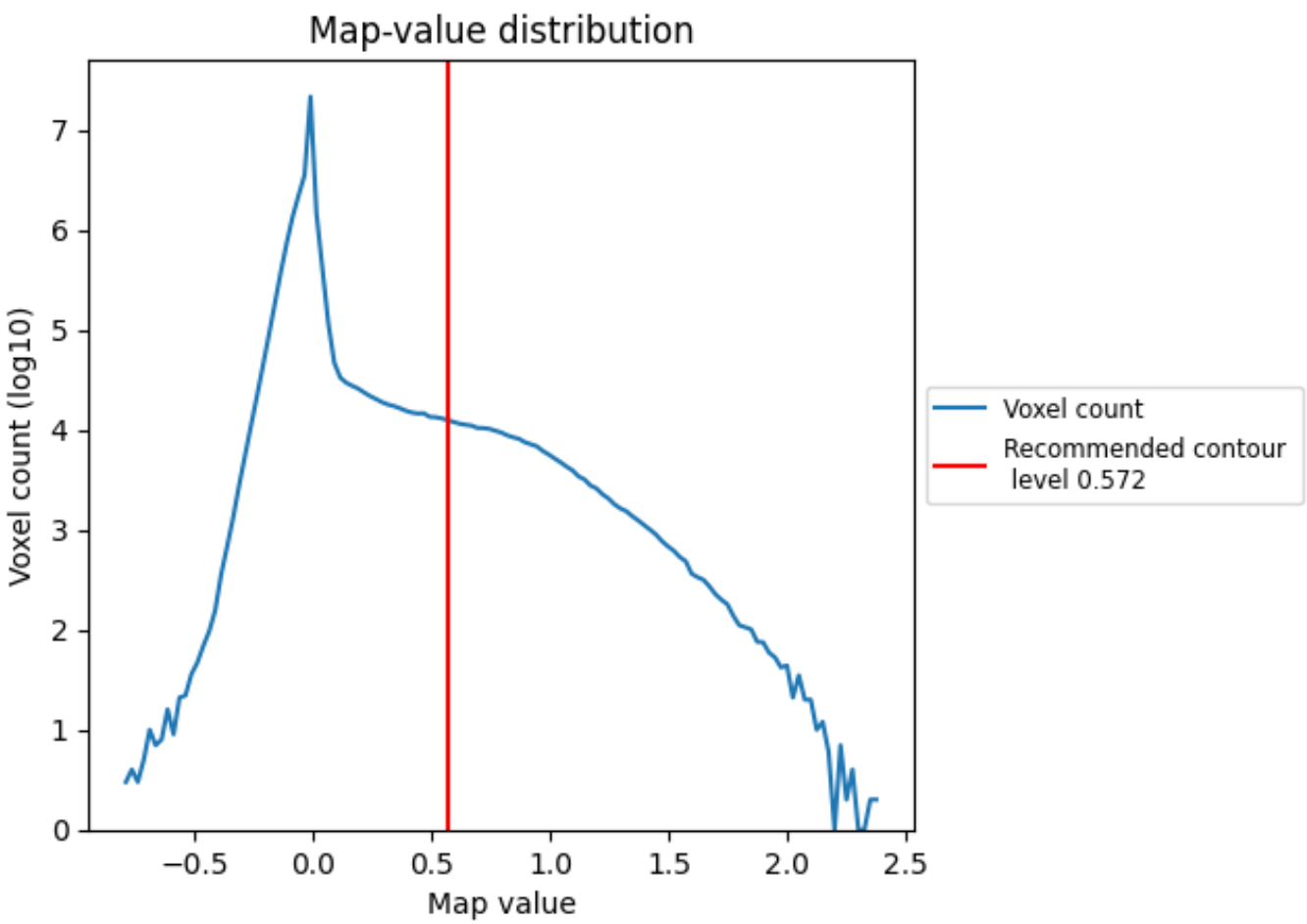
6.5 Mask visualisation (i)

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

7 Map analysis (i)

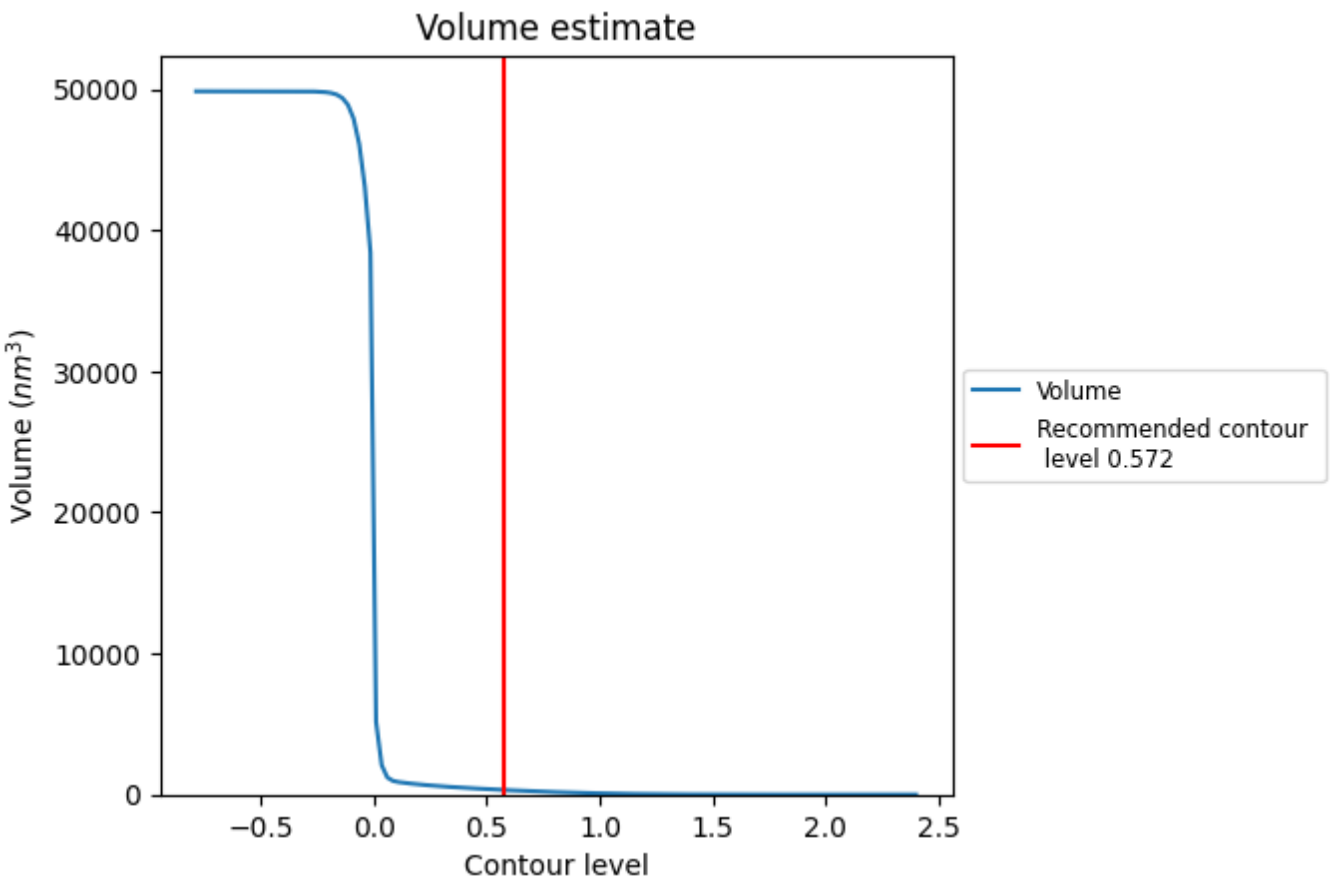
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

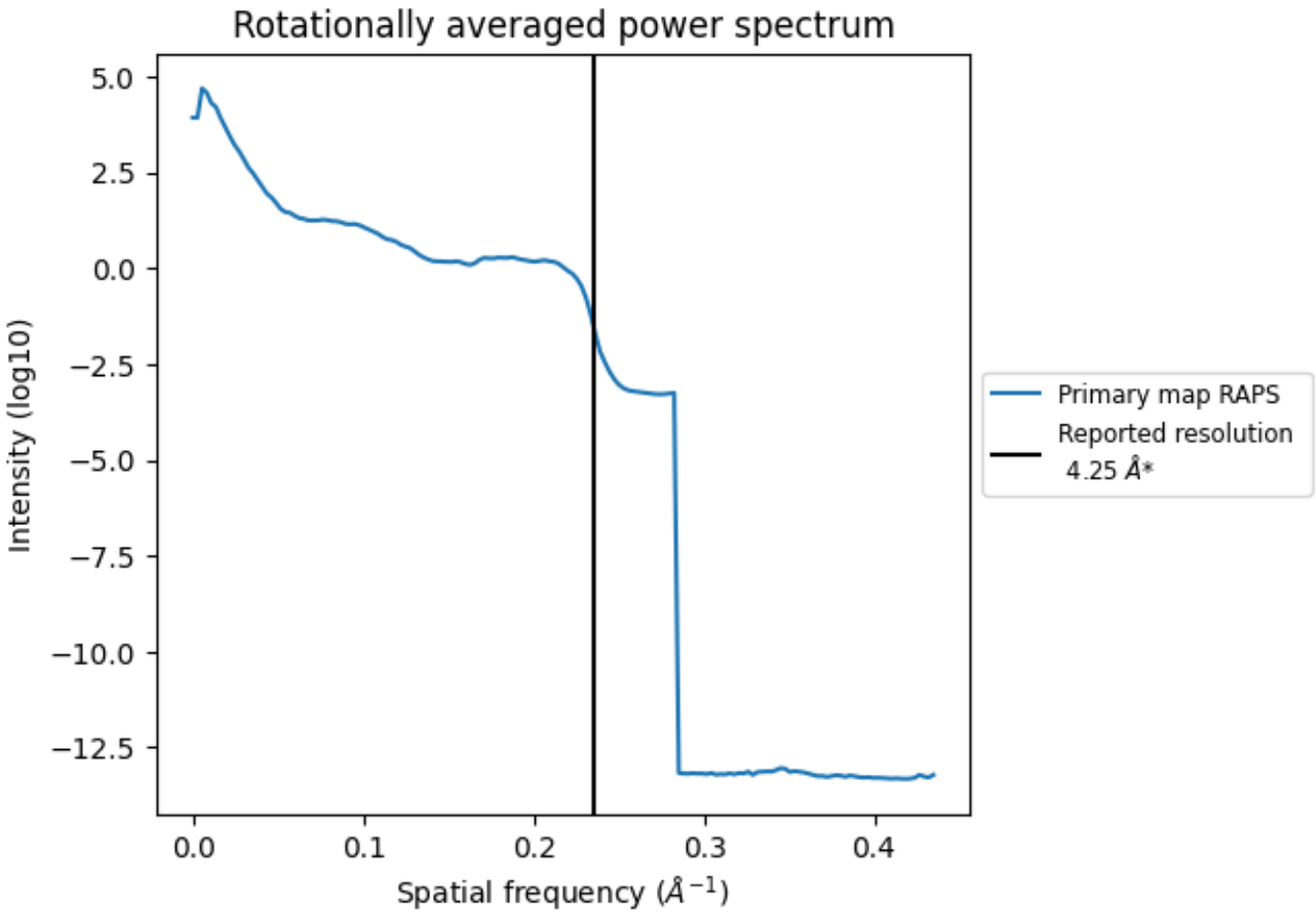
7.2 Volume estimate (i)



The volume at the recommended contour level is 330 nm^3; this corresponds to an approximate mass of 298 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)

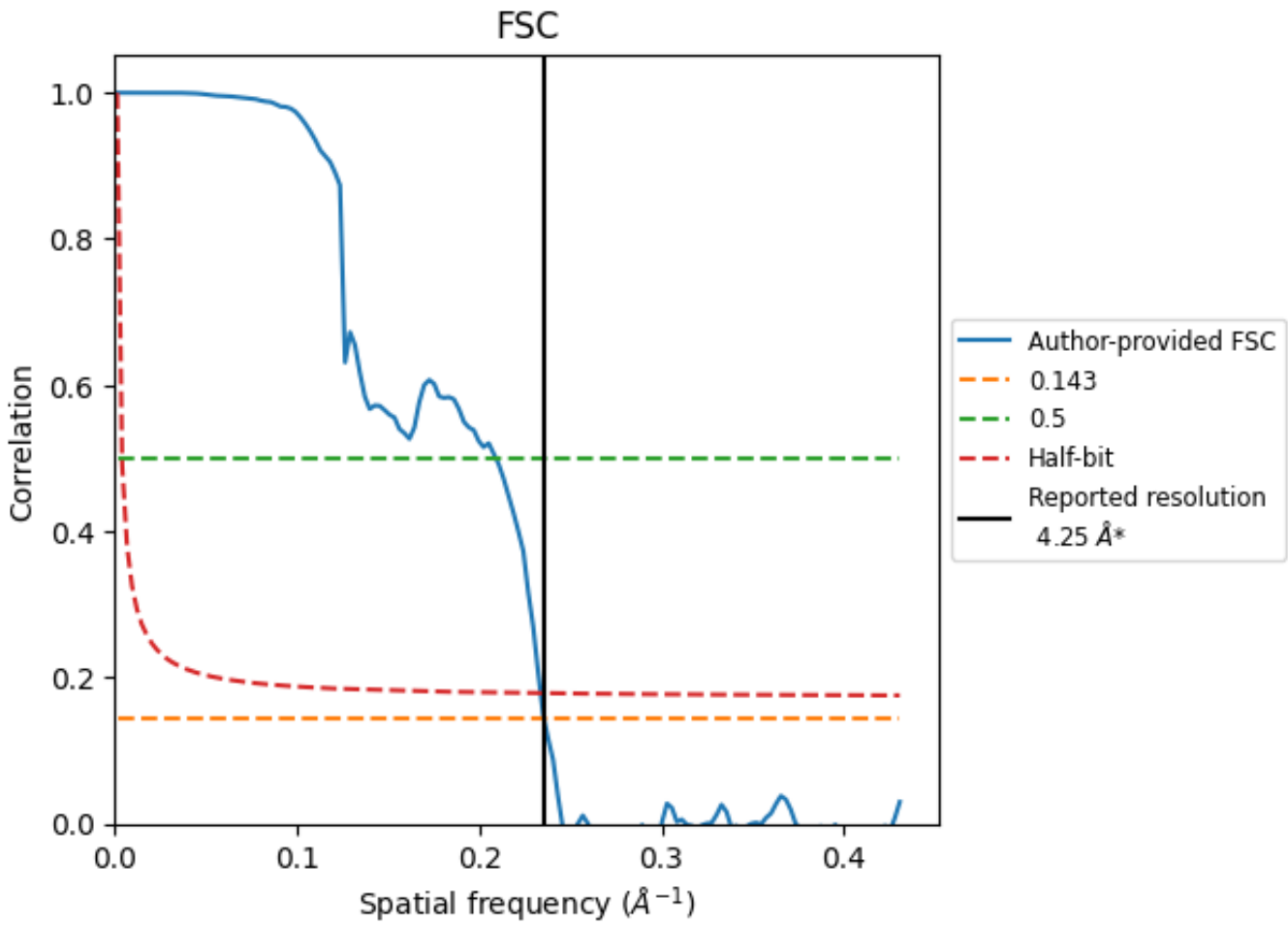


*Reported resolution corresponds to spatial frequency of 0.235 Å^{-1}

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 0.235 Å^{-1}

8.2 Resolution estimates (i)

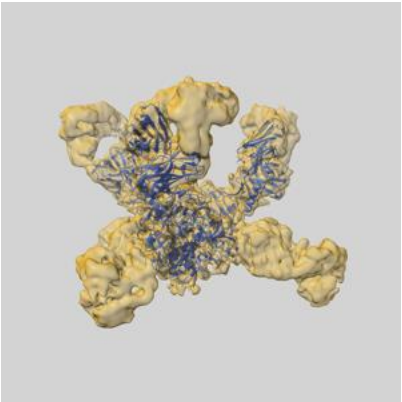
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.25	-	-
Author-provided FSC curve	4.25	4.78	4.28
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

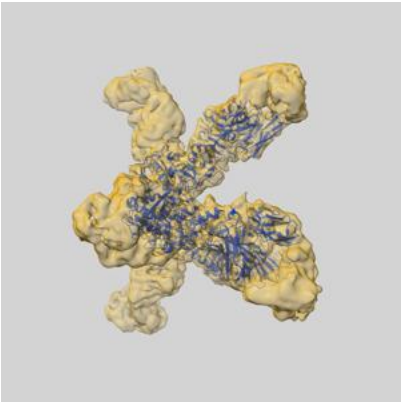
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-22842 and PDB model 7KEX. Per-residue inclusion information can be found in section 3 on page 12.

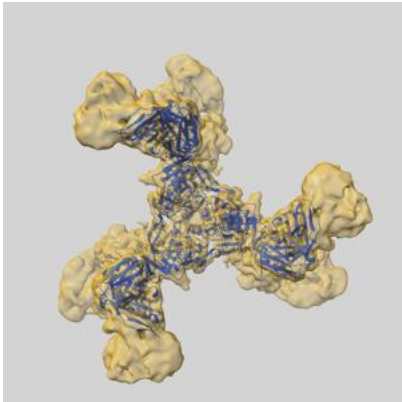
9.1 Map-model overlay (i)



X



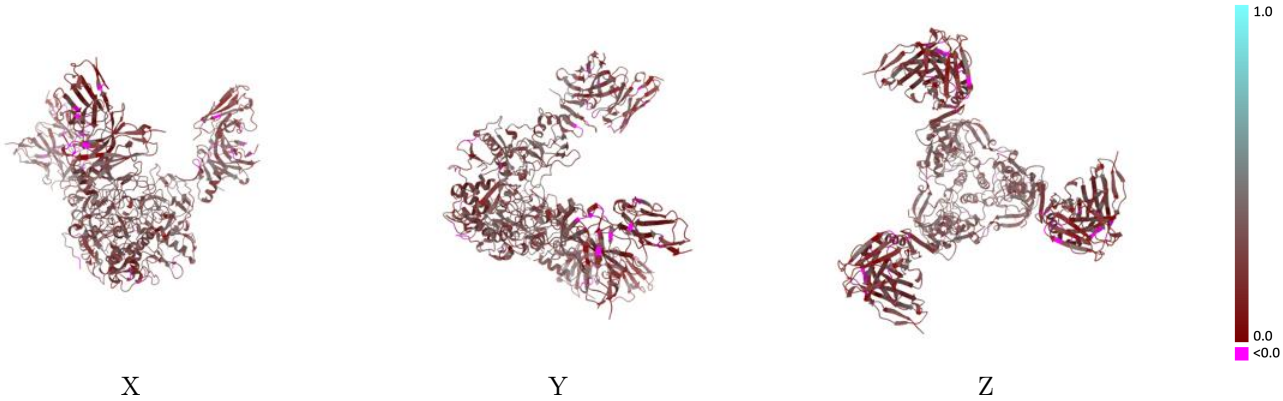
Y



Z

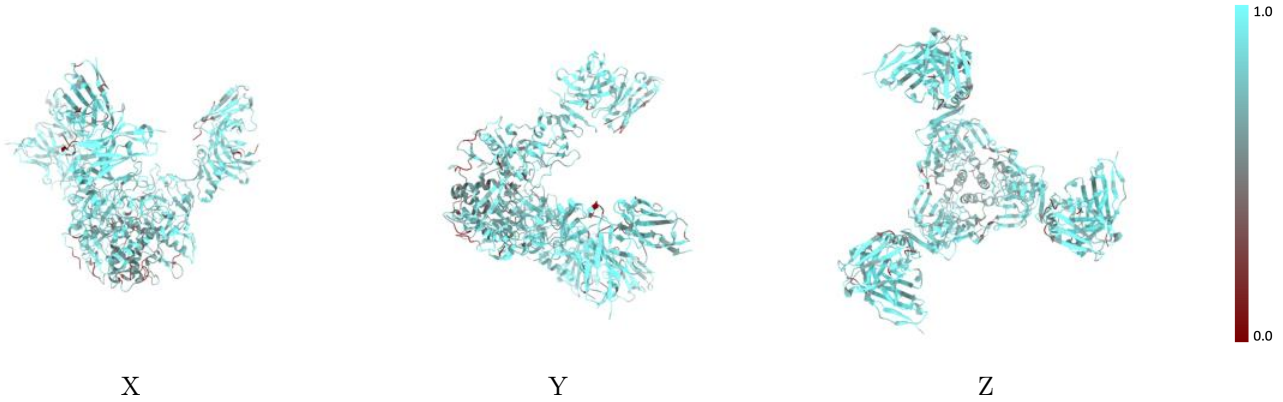
The images above show the 3D surface view of the map at the recommended contour level 0.572 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



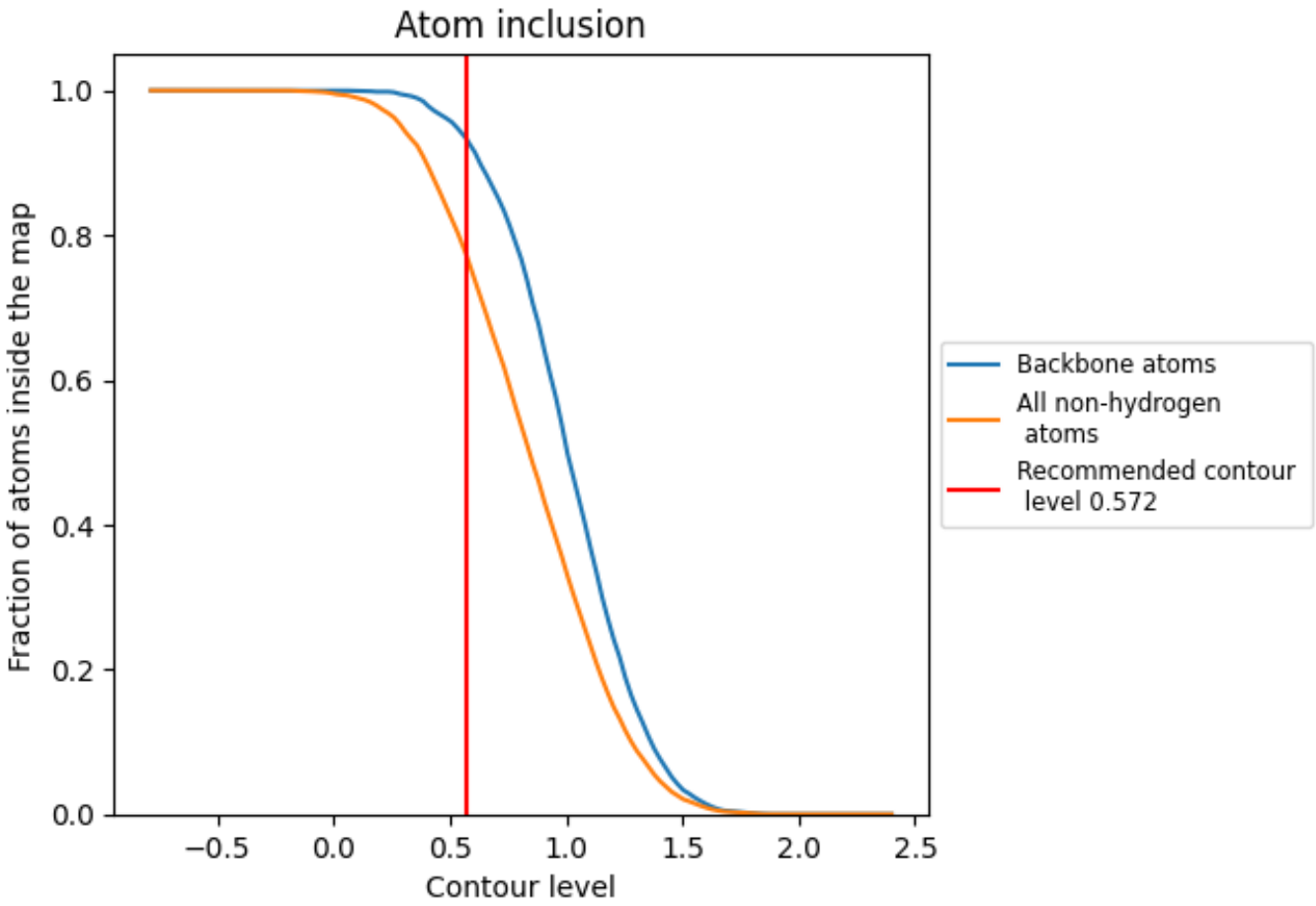
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.572).

9.4 Atom inclusion (i)



At the recommended contour level, 93% of all backbone atoms, 77% 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 (0.572) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7714	0.2560
A	0.7600	0.2870
B	0.7588	0.2840
C	0.7588	0.2850
D	0.7330	0.2650
E	0.7260	0.2660
F	0.7330	0.2660
G	0.8505	0.2370
H	0.8527	0.2410
I	0.8505	0.2400
J	0.7755	0.1980
K	0.7793	0.1950
L	0.7806	0.1940
M	0.4615	0.2610
N	0.4600	0.3390
O	0.4615	0.2810
P	0.4600	0.3410
Q	0.4615	0.2620
R	0.4600	0.3530